LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031122\
Data File : BP009375.D
Acq On : 11 Mar 2022 20:54
Operator : CG/JU
Sample : N1886-03 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
30969

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009375.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.064	10	13	22	rVB	198943	303061	1.62%	0.147%
2	3.658	106	114	127	rVB	468132	809655	4.32%	0.392%
3	4.087	161	187	189	rBV	699036	3051806	16.29%	1.477%
4	4.805	294	309	316	rBV	386177	1015866	5.42%	0.492%
5	4.946	322	333	343	rVB	305466	689959	3.68%	0.334%
6	5.111	354	361	378	rBV	2161360	3752149	20.02%	1.816%
7	5.381	396	407	410	rBV	136639	307807	1.64%	0.149%
8	5.434	410	416	424	rVB2	308338	676431	3.61%	0.327%
9	5.916	490	498	512	rVB	458837	807031	4.31%	0.391%
10	6.481	588	594	610	rVB	785170	1328574	7.09%	0.643%
11	6.922	655	669	679	rBV	403435	1130774	6.03%	0.547%
12	7.022	679	686	688	rBV	115957	210389	1.12%	0.102%
13	7.681	782	798	803	rBV	124755	369505	1.97%	0.179%
14	7.816	816	821	829	rVB	1258936	2159382	11.52%	1.045%
15	7.899	829	835	848	rBV	656284	1530818	8.17%	0.741%
16	8.105	859	870	885	rVB	409150	1048927	5.60%	0.508%
17	8.487	923	935	944	rBV	331194	839652	4.48%	0.406%
18	8.610	944	956	967	rVB	1018138	2346852	12.52%	1.136%
19	8.846	989	996	1001	rBV	348957	673505	3.59%	0.326%
20	8.969	1012	1017	1024	rVB	322483	584958	3.12%	0.283%
21	9.052	1024	1031	1047	rBV3	568234	1909214	10.19%	0.924%
22	9.246	1048	1064	1070	rBV	1104233	4603468	24.57%	2.228%
23	9.316	1071	1076	1098	rVB5	648896	2434480	12.99%	1.178%
24	9.493	1098	1106	1108	rBV2	686450	1387698	7.41%	0.672%
25	9.557	1109	1117	1118	rBV3	1157863	2205902	11.77%	1.068%
26	10.034	1190	1198	1200	rVV2	466399	903214	4.82%	0.437%
27	10.104	1200	1210	1214	rVB	1491206	3808668	20.32%	1.844%
28	10.163	1214	1220	1227	rVB2	230085	443946	2.37%	0.215%
29	10.252	1227	1235	1240	rBV3	343129	719888	3.84%	0.348%
30	10.357	1248	1253	1258	rBV6	107773	259274	1.38%	0.126%
31	10.446	1258	1268	1275	rVV2	764898	1946617	10.39%	0.942%
32	10.557	1279	1287	1292	rVV2	1056035	2269323	12.11%	1.098%
33	10.616	1292	1297	1303	rVB	1733532	3150216	16.81%	1.525%
34	10.687	1303	1309	1313	rBV	2521856	5405464	28.85%	2.617%
35	10.734	1313	1317	1324	rVB	1980844	3307531	17.65%	1.601%
36	10.816	1325	1331	1343	rVB4	594060	1327414	7.08%	0.643%

LSC Area Percent Report

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Acq On : 11 Mar 2022 20:54
Operator : CG/JU
Sample : N1886-03 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
30969

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.034	1343	1368	1372	rBV3	3341682	16374567	87.38%	7.926%
38	11.181	1382	1393	1398	rBV	9475282	18739620	100.00%	9.071%
39	11.240	1398	1403	1409	rVV	6909421	11704755	62.46%	5.666%
40	11.310	1409	1415	1419	rVV	1011009	2010692	10.73%	0.973%
41	11.346	1419	1421	1426	rVB	179001	238283	1.27%	0.115%
42	11.399	1426	1430	1434	rBV3	128869	197066	1.05%	0.095%
43	11.475	1434	1443	1446	rBV6	544479	1588528	8.48%	0.769%
44	11.551	1447	1456	1460	rVV5	1520406	4097718	21.87%	1.984%
45	11.599	1460	1464	1468	rVB	556459	778828	4.16%	0.377%
46	11.699	1475	1481	1484	rBV2	725193	1481063	7.90%	0.717%
47	11.781	1490	1495	1497	rBV5	498797	946739	5.05%	0.458%
48	11.834	1502	1504	1508	rVB	1535330	1884757	10.06%	0.912%
49	11.875	1508	1511	1519	rVB5	415648	750981	4.01%	0.364%
50	11.981	1519	1529	1535	rVB2	1283934	3106230	16.58%	1.504%
51	12.040	1535	1539	1541	rBV2	345183	523146	2.79%	0.253%
52	12.075	1541	1545	1548	rBV3	546831	955699	5.10%	0.463%
53	12.116	1548	1552	1560	rVB3	1187910	3148399	16.80%	1.524%
54	12.193	1560	1565	1572	rVB2	608464	1088637	5.81%	0.527%
55	12.287	1572	1581	1592	rBV6	1395395	4646431	24.79%	2.249%
56	12.381	1592	1597	1605	rVB6	314813	786091	4.19%	0.381%
57	12.498	1614	1617	1623	rVB2	263879	435867	2.33%	0.211%
58	12.563	1623	1628	1634	rBV4	277990	555913	2.97%	0.269%
59	12.704	1647	1652	1660	rVB2	251279	498324	2.66%	0.241%
60	12.810	1661	1670	1676	rBV	1163650	2133638	11.39%	1.033%
61	12.898	1680	1685	1693	rVB3	260989	494942	2.64%	0.240%
62	13.081	1711	1716	1729	rVB	877294	1883248	10.05%	0.912%
63	13.234	1737	1742	1746	rBV	189620	321809	1.72%	0.156%
64	13.434	1771	1776	1784	rBV6	241925	622717	3.32%	0.301%
65	13.557	1794	1797	1802	rVB2	159002	228236	1.22%	0.110%
66	13.922	1853	1859	1866	rBV3	581894	1094893	5.84%	0.530%
67	13.987	1866	1870	1874	rBV	192093	281041	1.50%	0.136%
68	14.128	1889	1894	1901	rBV3	152891	298524	1.59%	0.145%
69	14.216	1903	1909	1916	rBV2	794739	1536880	8.20%	0.744%
70	14.310	1917	1925	1929	rBV3	312419	592718	3.16%	0.287%
71	14.392	1934	1939	1944	rVV3	301136	603529	3.22%	0.292%
72	14.457	1944	1950	1959	rVV	2591394	4637956	24.75%	2.245%
73	14.540	1959	1964	1973	rVB2	315693	612718	3.27%	0.297%
74	14.704	1987	1992	1999	rBV2	336670	747129	3.99%	0.362%
75	14.775	2000	2004	2014	rVB3	152274	394822	2.11%	0.191%
76	14.910	2024	2027	2034	rVB	226448	301162	1.61%	0.146%

LSC Area Percent Report

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Misc :
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Instrument :
BNA_P
ClientSampleId :
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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	15.198	2072	2076	2079	rBV4	112391	228243	1.22%	0.110%
78	15.704	2158	2162	2170	rVB3	144362	264398	1.41%	0.128%
79	15.957	2200	2205	2213	rBV	631090	1042113	5.56%	0.504%
80	16.881	2359	2362	2366	rVB2	174787	246601	1.32%	0.119%
81	17.034	2382	2388	2394	rVB	5325373	7802433	41.64%	3.777%
82	17.163	2405	2410	2415	rBV	2186098	3076780	16.42%	1.489%
83	17.222	2415	2420	2429	rVB	3072399	4656639	24.85%	2.254%
84	17.333	2434	2439	2447	rVB	1551428	2229940	11.90%	1.079%
85	17.433	2451	2456	2461	rBV	976876	1366107	7.29%	0.661%
86	17.498	2462	2467	2471	rBV2	603615	878636	4.69%	0.425%
87	17.845	2522	2526	2532	rBV	573296	828541	4.42%	0.401%
88	18.016	2551	2555	2561	rBV	170407	259101	1.38%	0.125%
89	18.133	2571	2575	2579	rBV	233106	348628	1.86%	0.169%
90	19.304	2771	2774	2778	rVB	617720	698110	3.73%	0.338%
91	19.792	2854	2857	2866	rVB	1221822	1618162	8.63%	0.783%
92	21.327	3114	3118	3126	rVB	3632958	5294675	28.25%	2.563%
93	21.457	3135	3140	3156	rVB	11785331	17524410	93.52%	8.483%
94	23.745	3523	3529	3537	rBV2	2502554	5179562	27.64%	2.507%

Sum of corrected areas: 206586793

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031122\
Data File : BP009375.D
Acq On : 11 Mar 2022 20:54
Operator : CG/JU
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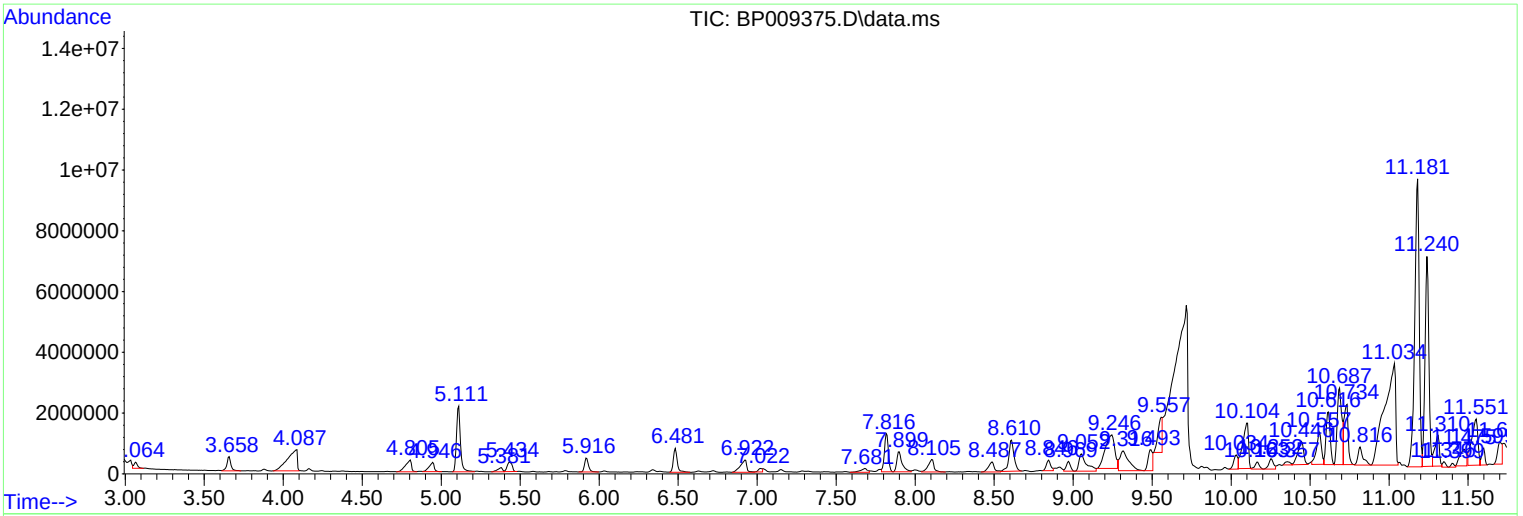
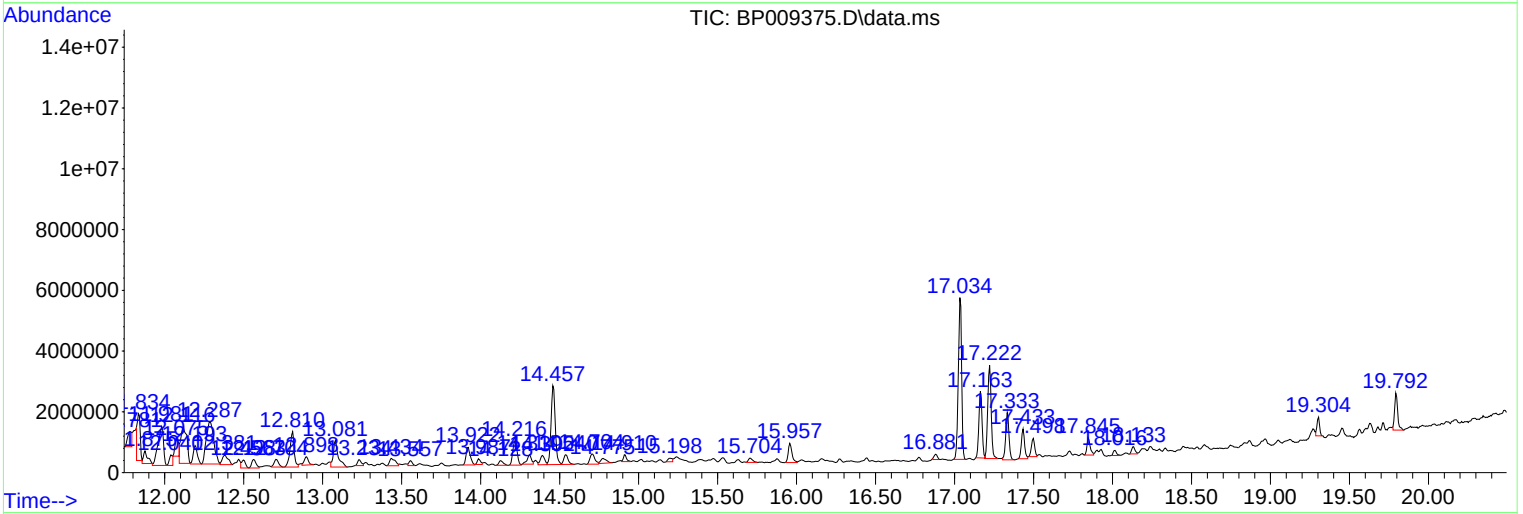
Misc :
ALS Vial : 18 Sample Multiplier: 1

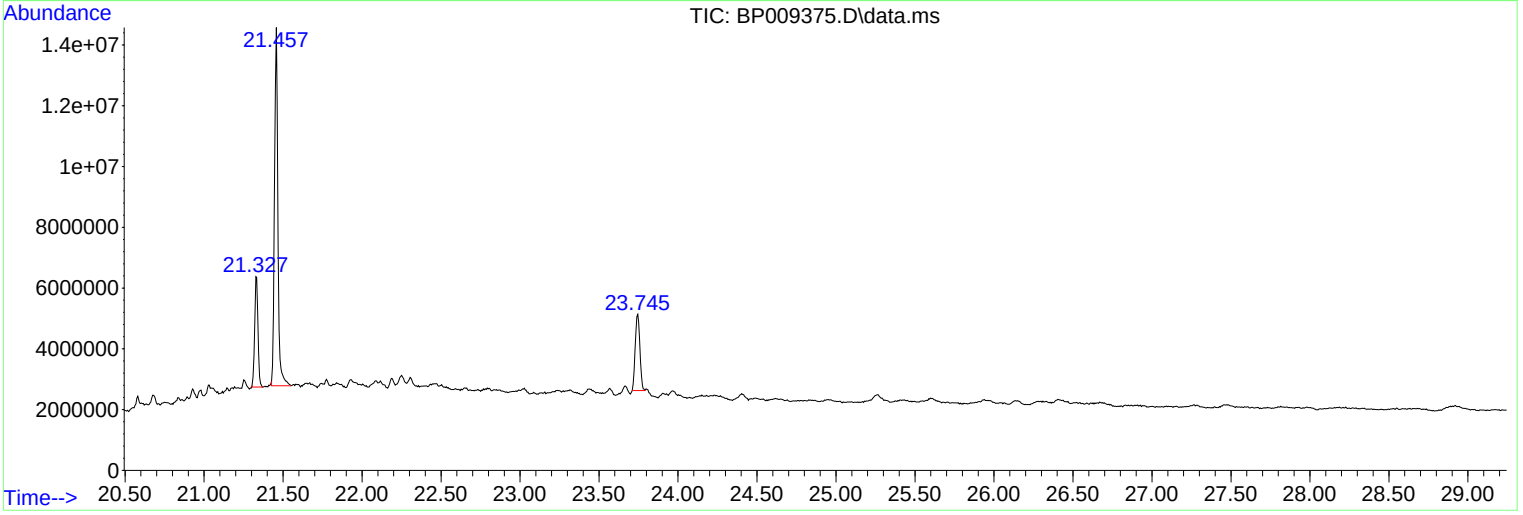
Instrument :
BNA_P
ClientSampleId :
30969

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031122\
Data File : BP009375.D
Acq On : 11 Mar 2022 20:54
Operator : CG/JU
Sample : N1886-03 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
30969

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

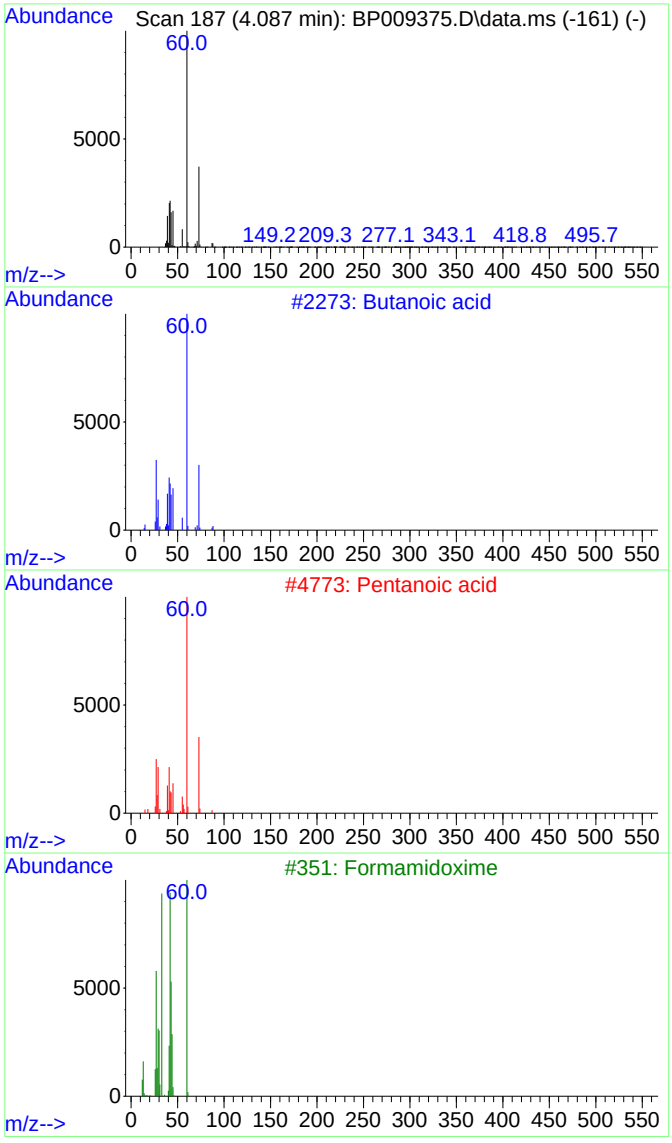
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

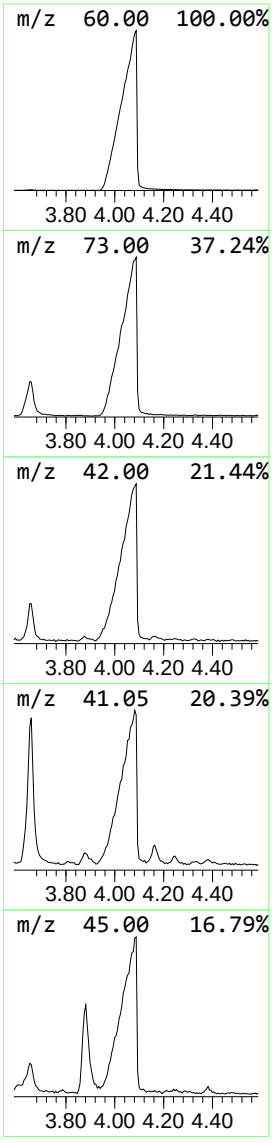
****

Peak Number 1 Butanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.087	28.27 ng	3051810	1,4-Dichlorobenzene-d4	7.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	91
2	Pentanoic acid	102	C5H10O2	000109-52-4	40
3	Formamidoxime	60	CH4N2O	000624-82-8	9
4	Hexanoic acid	116	C6H12O2	000142-62-1	9
5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031122\
Data File : BP009375.D
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

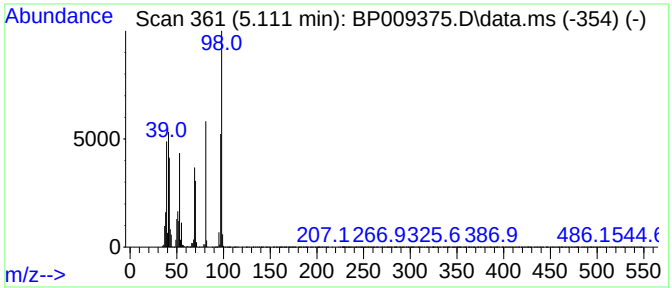
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

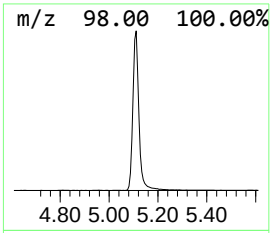
****

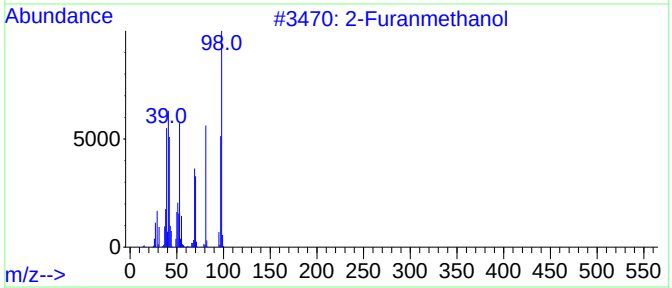
Peak Number 2 2-Furanmethanol Concentration Rank 5

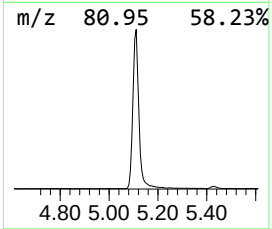
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.111	34.75 ng	3752150	1,4-Dichlorobenzene-d4	7.816

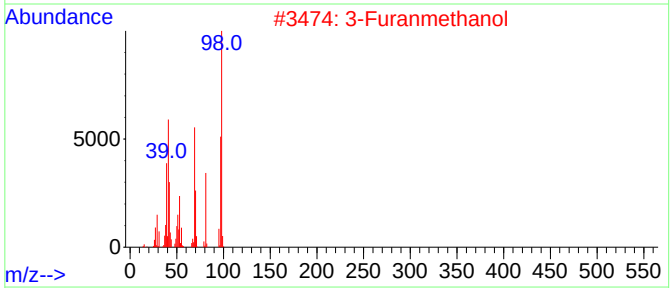
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Furanmethanol	98	C5H6O2	000098-00-0	98
2	3-Furanmethanol	98	C5H6O2	004412-91-3	60
3	Methylenecyclopropanecarboxylic ...	98	C5H6O2	062266-36-8	50
4	6-Methoxy-2,6-dihydropyran-3-one	128	C6H8O3	1000411-44-4	38
5	3H-Pyrazol-3-one, 2,4-dihydro-5-...	98	C4H6N2O	000108-26-9	35

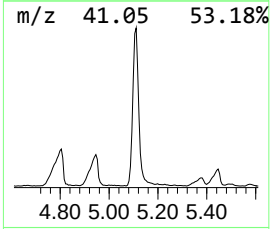


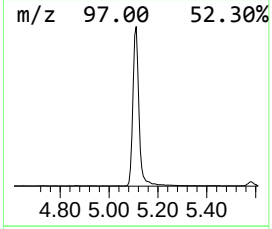


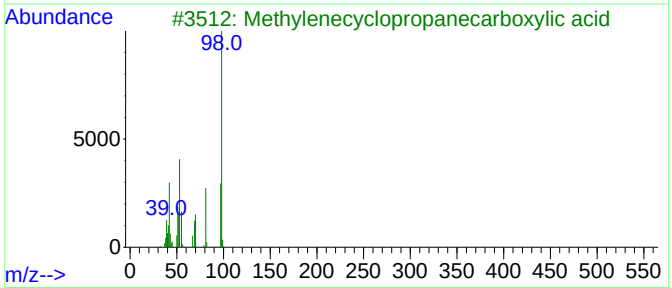


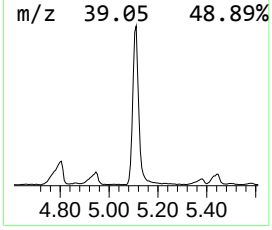












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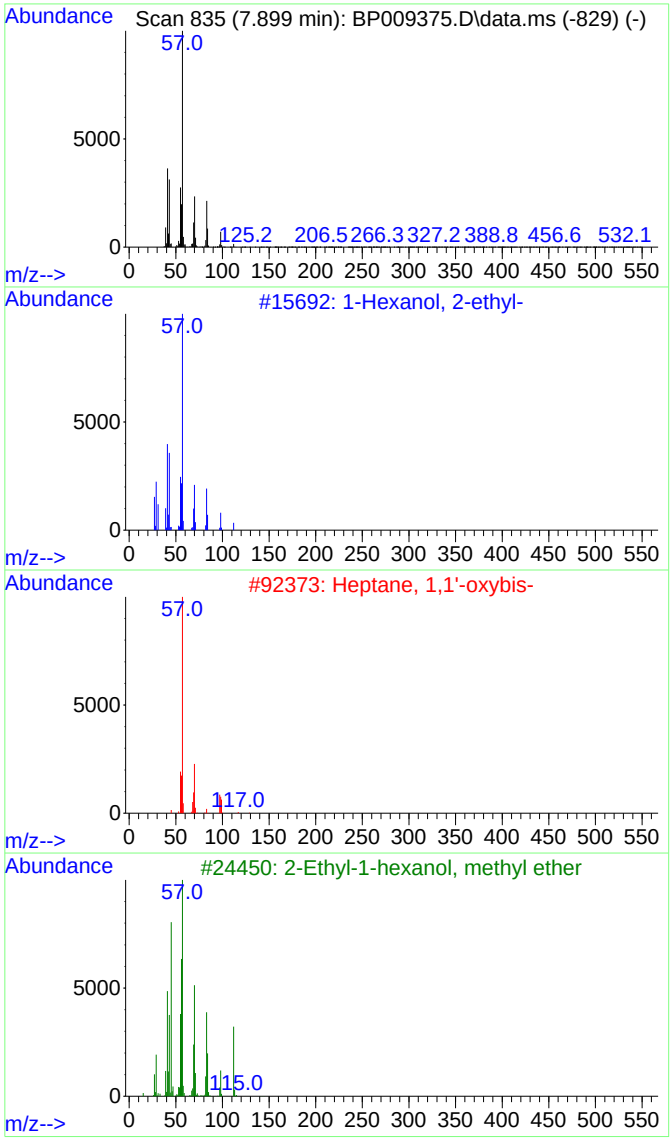
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

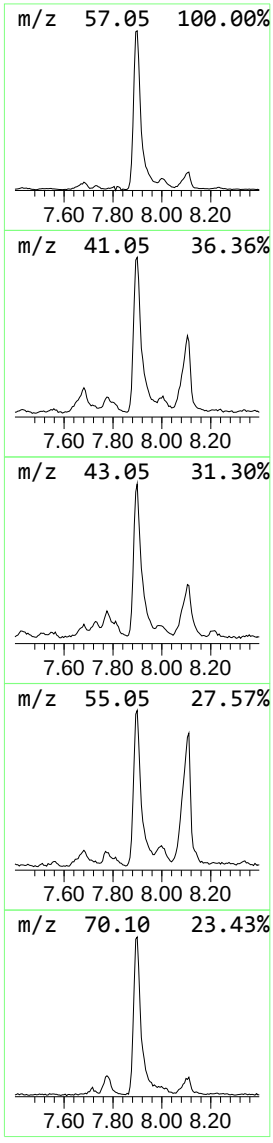
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.899	14.18 ng	1530820	1,4-Dichlorobenzene-d4	7.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
3	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
4	Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	47
5	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031122\
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

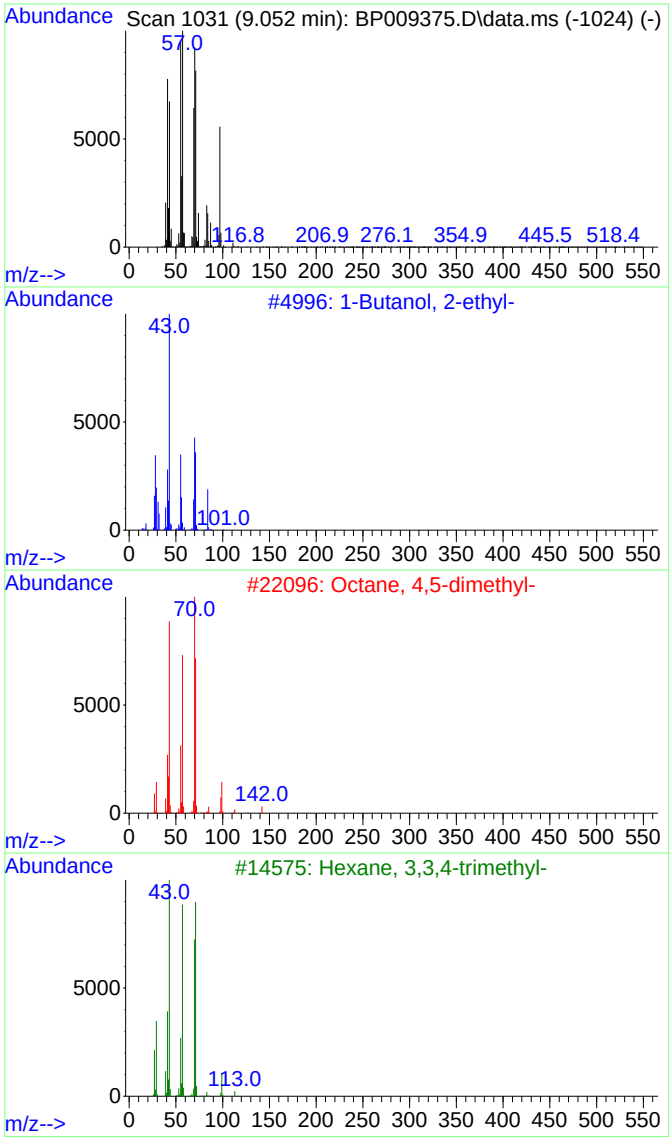
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

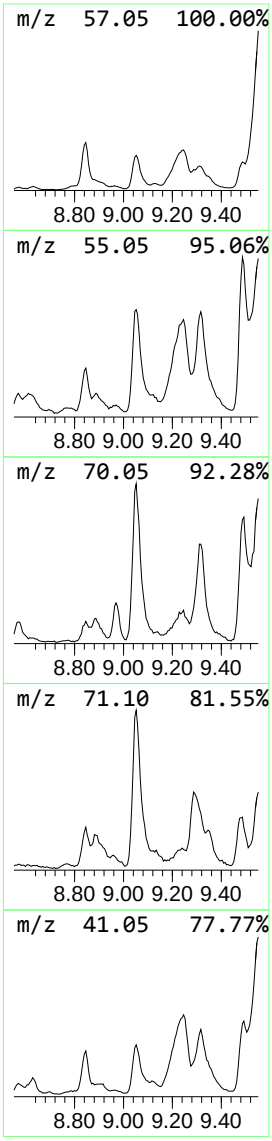
****

Peak Number 4 1-Butanol, 2-ethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.052	17.68 ng	1909210	1,4-Dichlorobenzene-d4	7.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	53
2	Octane, 4,5-dimethyl-	142	C10H22	015869-96-2	47
3	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	47
4	Isopentyl propyl carbonate	174	C9H18O3	1000373-84-4	43
5	1-Hexene, 3,5,5-trimethyl-	126	C9H18	004316-65-8	43





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Acq On : 11 Mar 2022 20:54
Operator : CG/JU
Sample : N1886-03 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
30969

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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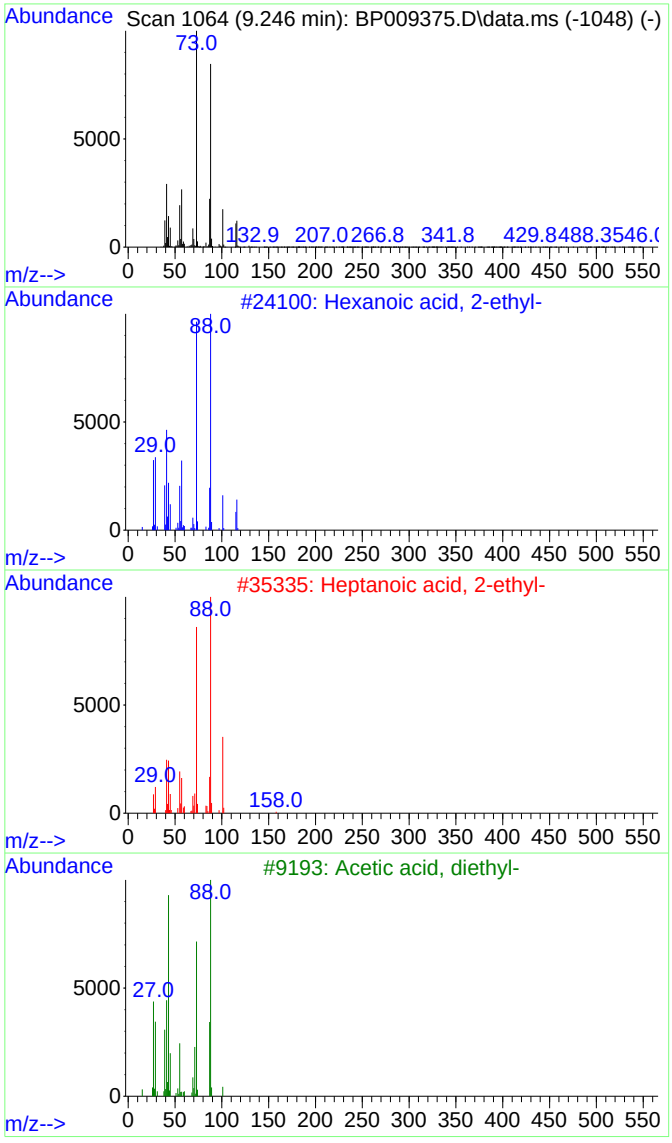
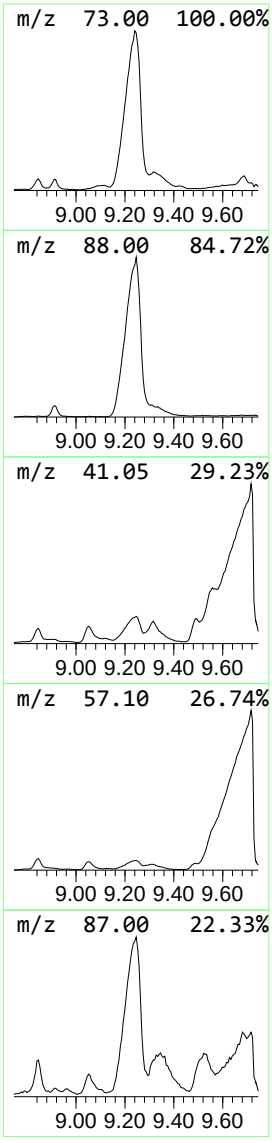
Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.246	29.23 ng	4603470	Naphthalene-d8	10.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	59
3	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	59
4	Octanoic acid, 2-methyl-, methyl...	172	C10H20O2	002177-86-8	38
5	1,4-Dioxane	88	C4H8O2	000123-91-1	37





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ALS Vial : 18 Sample Multiplier: 1

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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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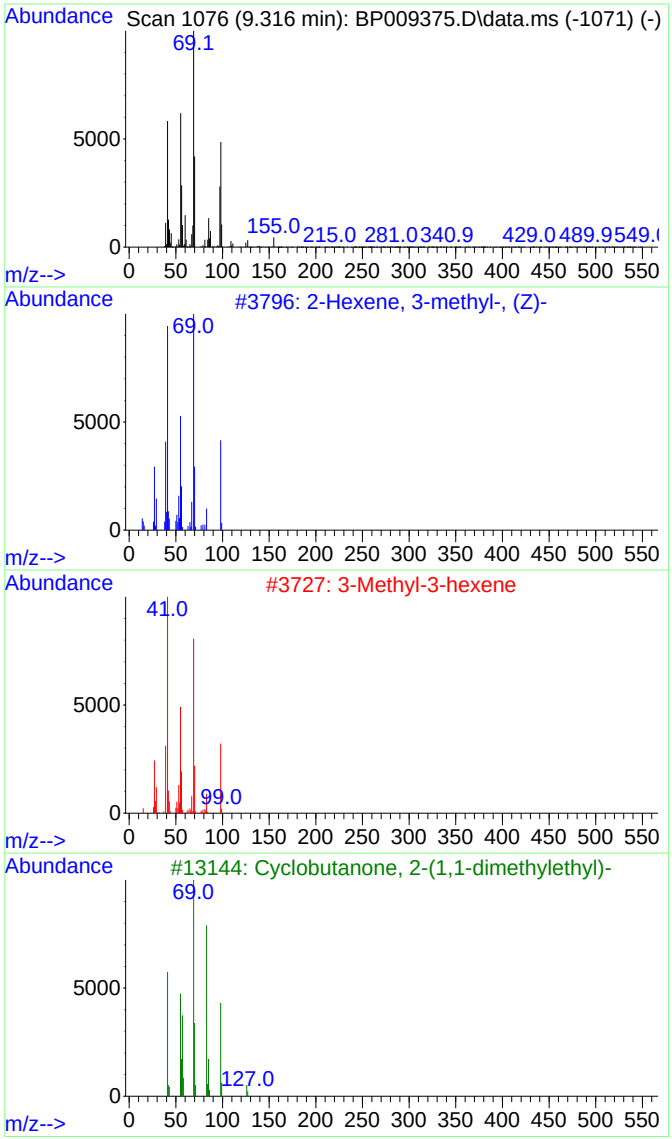
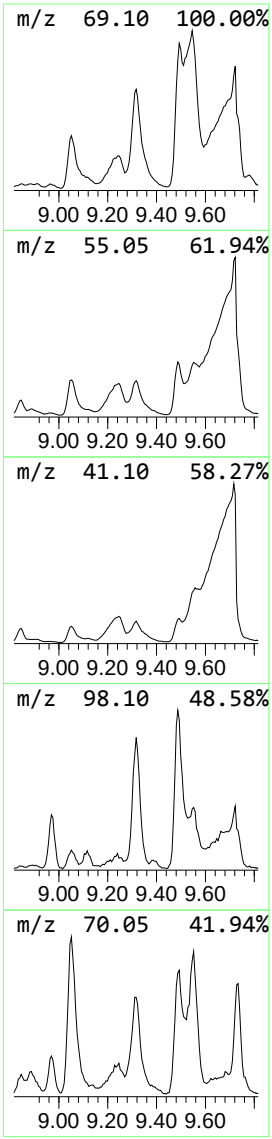
Peak Number 6 2-Hexene, 3-methyl-, (Z)- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.316	15.46 ng	2434480	Naphthalene-d8	10.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexene, 3-methyl-, (Z)-	98	C7H14	010574-36-4	53
2	3-Methyl-3-hexene	98	C7H14	003404-65-7	50
3	Cyclobutanone, 2-(1,1-dimethylet...	126	C8H14O	004579-31-1	50
4	1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	47
5	Cyclopropane, 1,1-dichloro-2-met...	194	C9H16Cl2	024551-82-4	42





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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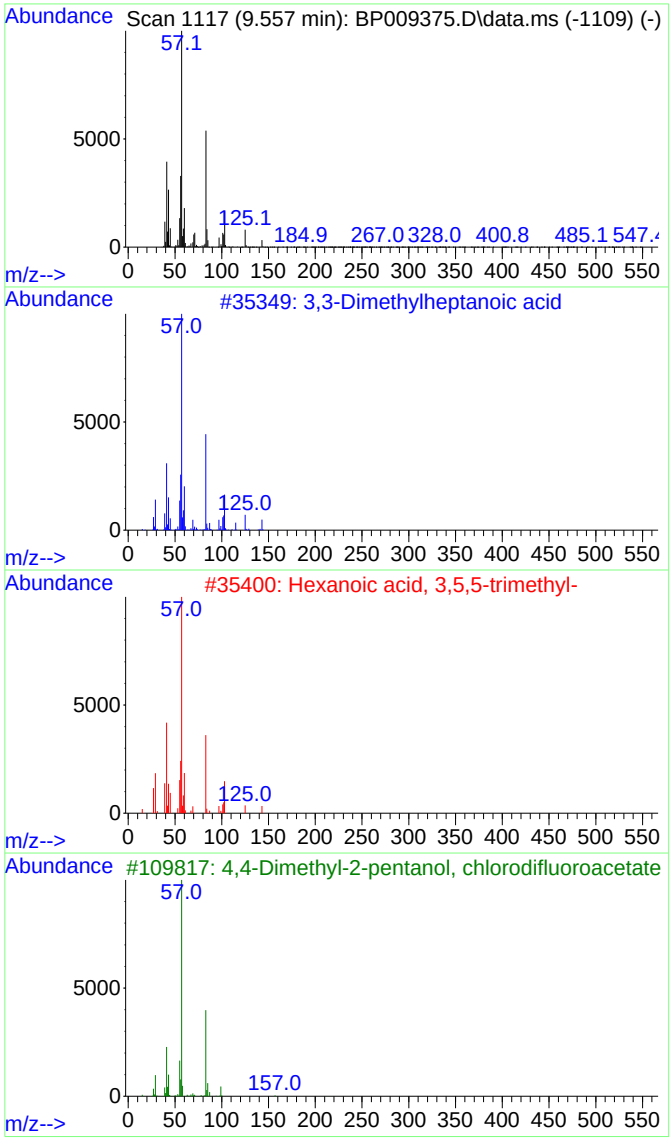
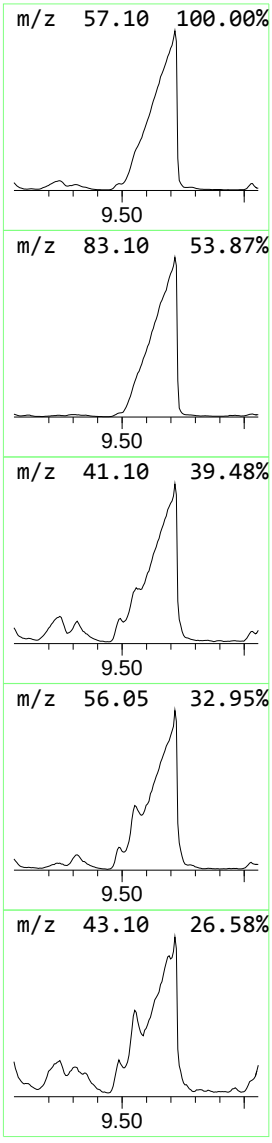
Peak Number 7 3,3-Dimethylheptanoic acid Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.557	14.00 ng	2205900	Naphthalene-d8	10.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	83
2	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	59
3	4,4-Dimethyl-2-pentanol, chlorod...	228	C9H15ClF2O2	1000376-27-0	43
4	1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	38
5	Imidazole, 2-acetamido-	125	C5H7N3O	052737-49-2	32





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Misc :
ALS Vial : 18 Sample Multiplier: 1

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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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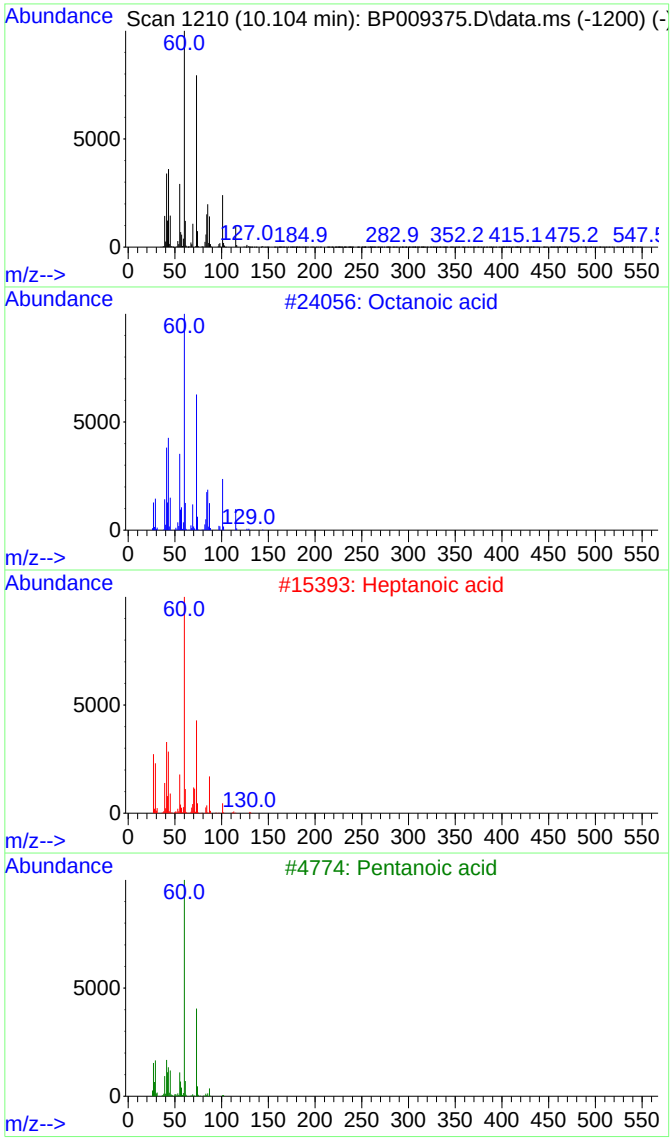
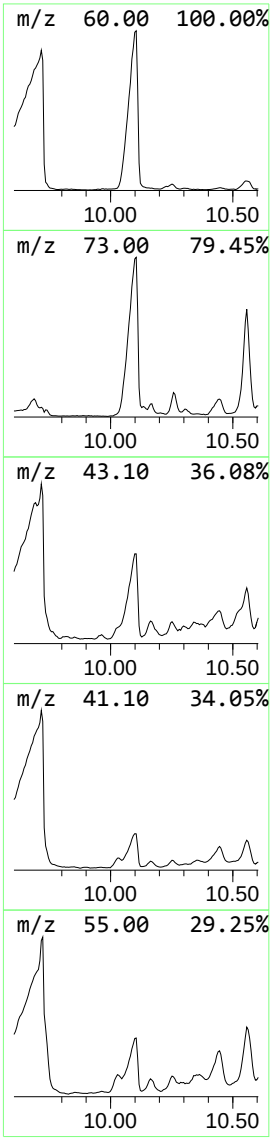
Peak Number 8 Octanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.105	24.18 ng	3808670	Naphthalene-d8	10.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	94
2	Heptanoic acid	130	C7H14O2	000111-14-8	53
3	Pentanoic acid	102	C5H10O2	000109-52-4	50
4	Hexanoic acid	116	C6H12O2	000142-62-1	46
5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	43





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Sample : N1886-03 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

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BNA_P
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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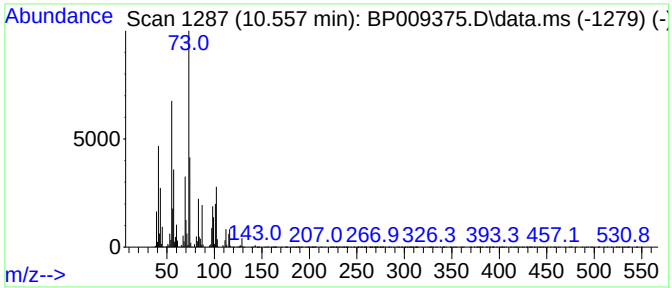
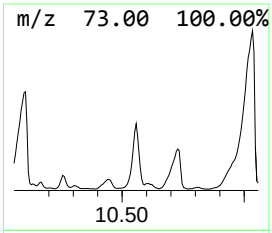
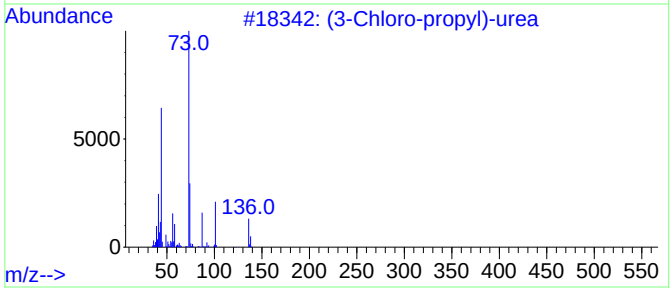
Peak Number 9 unknown10.557 Concentration Rank 18

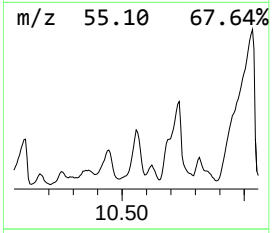
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.557	14.41 ng	2269320	Naphthalene-d8	10.610

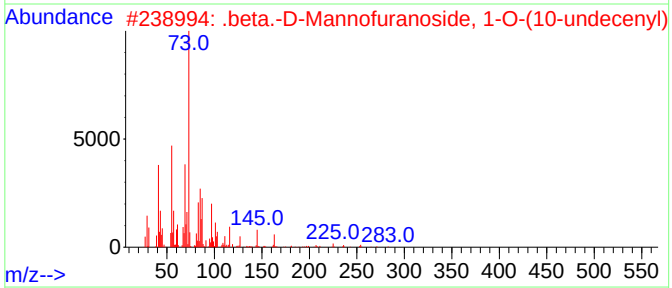
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3-Chloro-propyl)-urea	136	C4H9ClN2O	1000300-24-6	37
2	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	25
3	Nonanedioic acid, 4-oxo-, 9-meth...	216	C10H16O5	109300-55-2	17
4	Myo-Inositol, 4-C-methyl-	194	C7H14O6	000472-95-7	12
5	3,4-Dimethyl-3-hexanol	130	C8H18O	019550-08-4	12

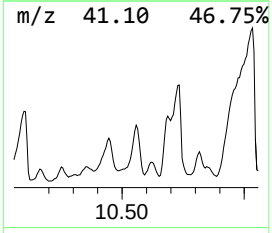


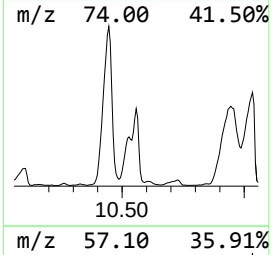


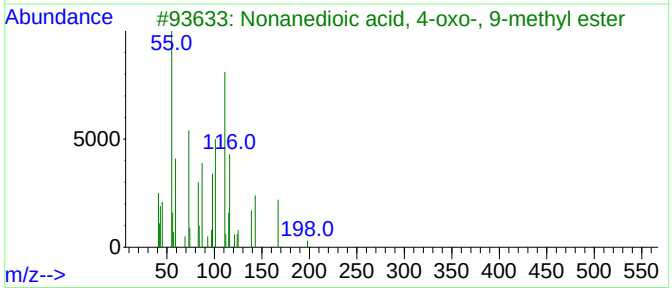


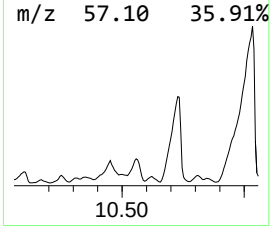












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Acq On : 11 Mar 2022 20:54
Operator : CG/JU
Sample : N1886-03 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
30969

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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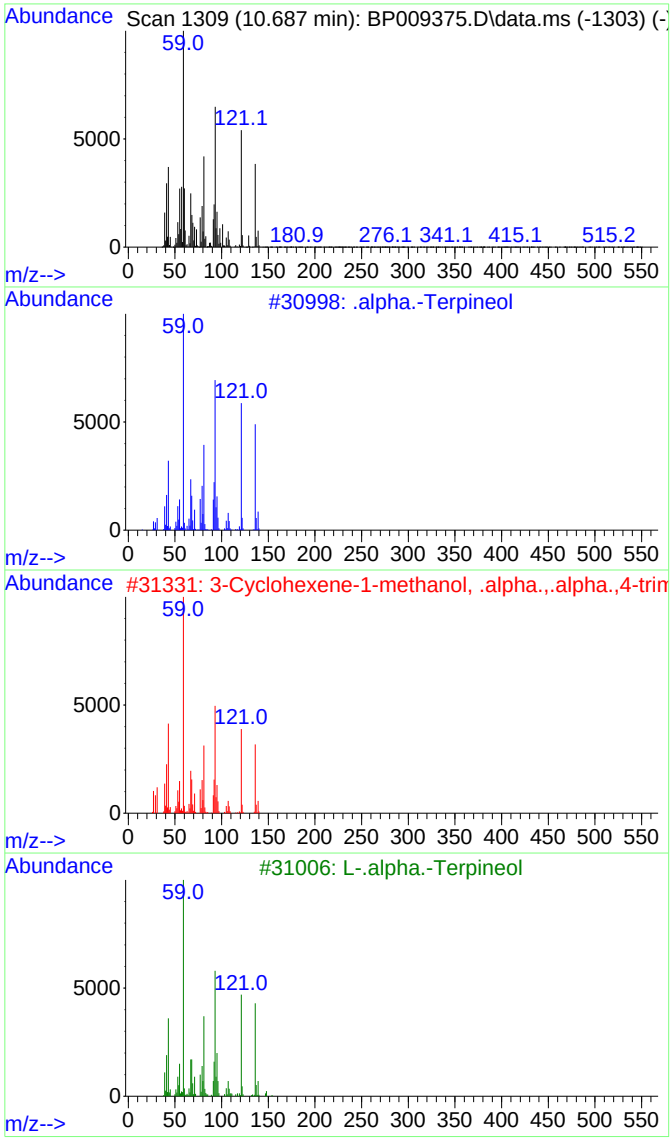
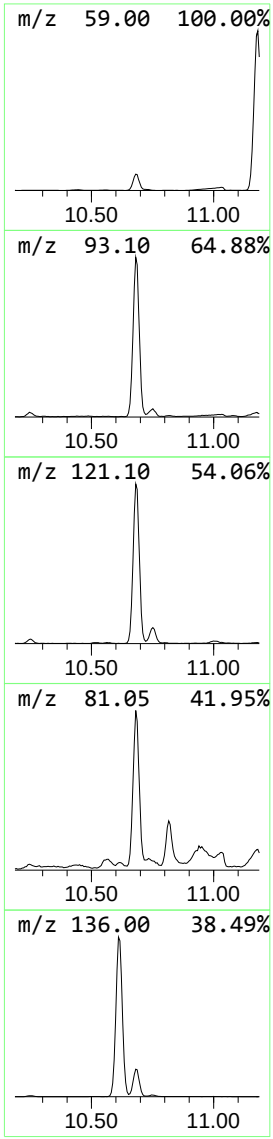
Peak Number 10 .alpha.-Terpineol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.687	34.32 ng	5405460	Naphthalene-d8	10.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Terpineol	154	C10H18O	000098-55-5	87
2	3-Cyclohexene-1-methanol, .alpha...	154	C10H18O	007785-53-7	83
3	L-.alpha.-Terpineol	154	C10H18O	010482-56-1	58
4	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	46
5	(+)-4-Carene	136	C10H16	029050-33-7	42





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Misc :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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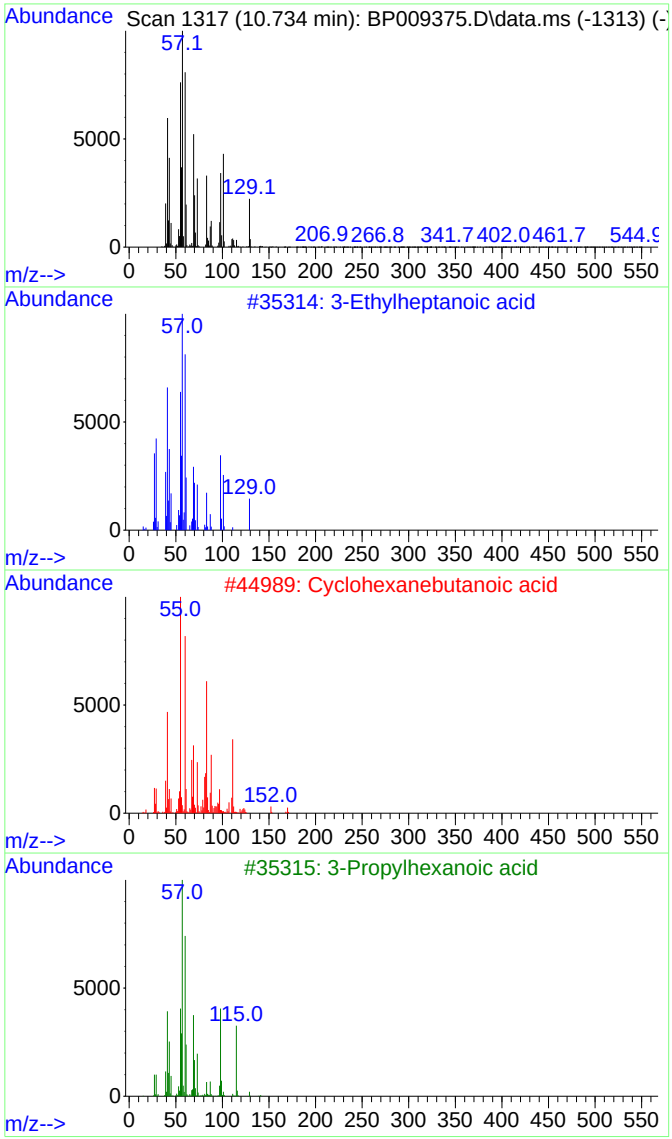
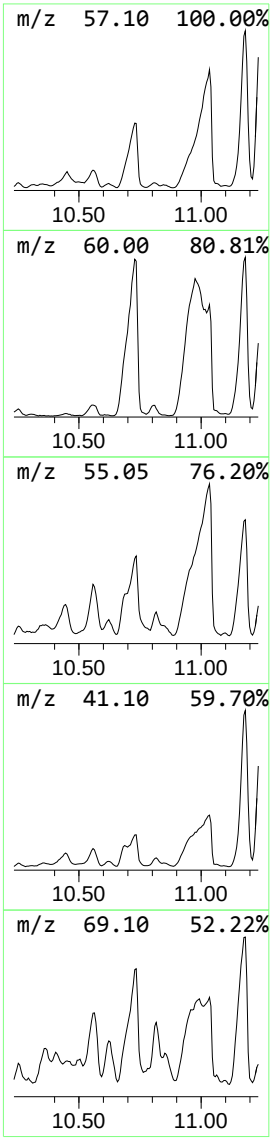
Peak Number 11 3-Ethylheptanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.734	21.00 ng	3307530	Naphthalene-d8	10.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Ethylheptanoic acid	158	C9H18O2	014272-47-0	50
2	Cyclohexanebutanoic acid	170	C10H18O2	004441-63-8	38
3	3-Propylhexanoic acid	158	C9H18O2	025110-61-6	37
4	Thiazole, 4,5-dihydro-2-methyl-	101	C4H7NS	002346-00-1	25
5	.alpha.-d-Ribopyranoside, methyl	164	C6H12O5	006207-03-0	25





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Misc :
ALS Vial : 18 Sample Multiplier: 1

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BNA_P
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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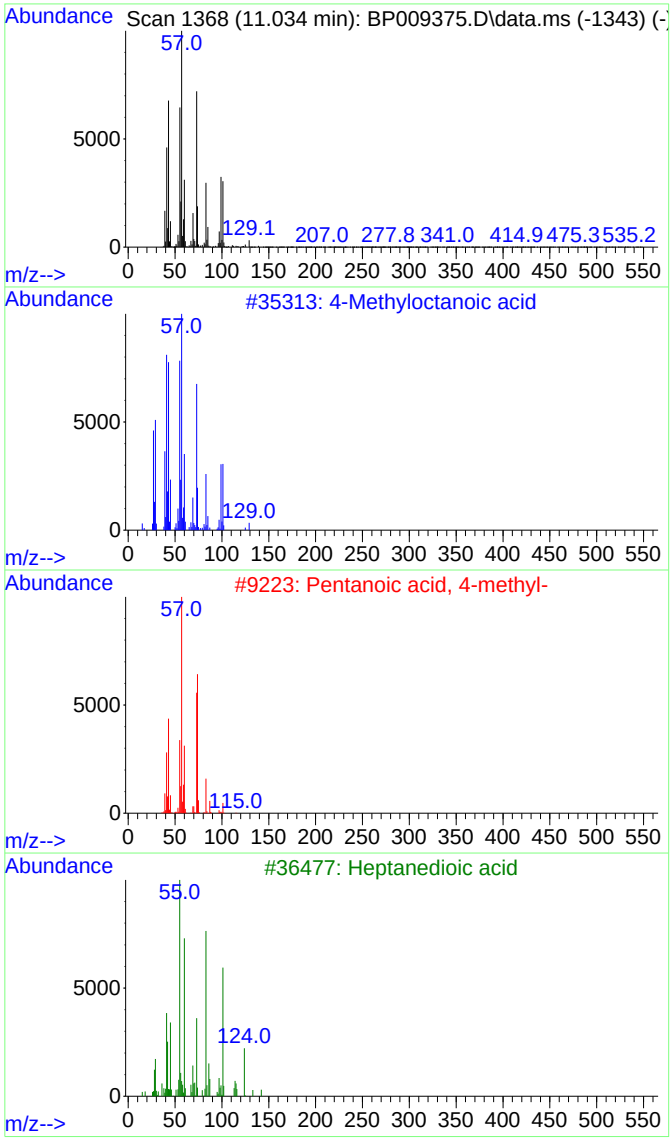
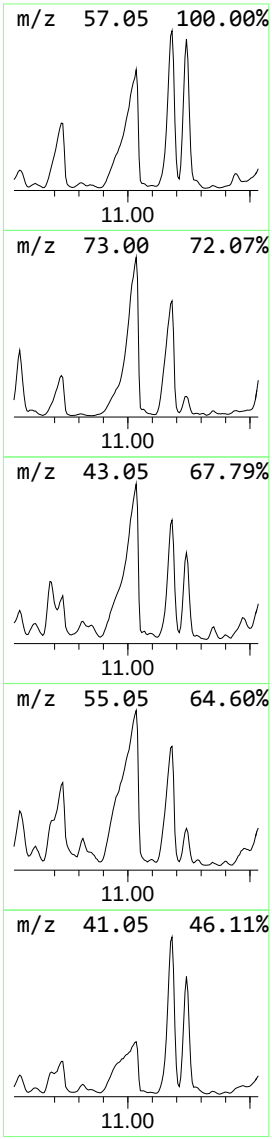
Peak Number 12 4-Methyloctanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.034	103.96 ng	16374600	Naphthalene-d8	10.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyloctanoic acid	158	C9H18O2	054947-74-9	86
2	Pentanoic acid, 4-methyl-	116	C6H12O2	000646-07-1	64
3	Heptanedioic acid	160	C7H12O4	000111-16-0	35
4	Cyclobutanecarboxylic acid, 2-bu...	156	C9H16O2	1000282-60-4	35
5	Pentanoic acid, 4,4-dimethyl-3-o...	158	C8H14O3	055107-14-7	27





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ALS Vial : 18 Sample Multiplier: 1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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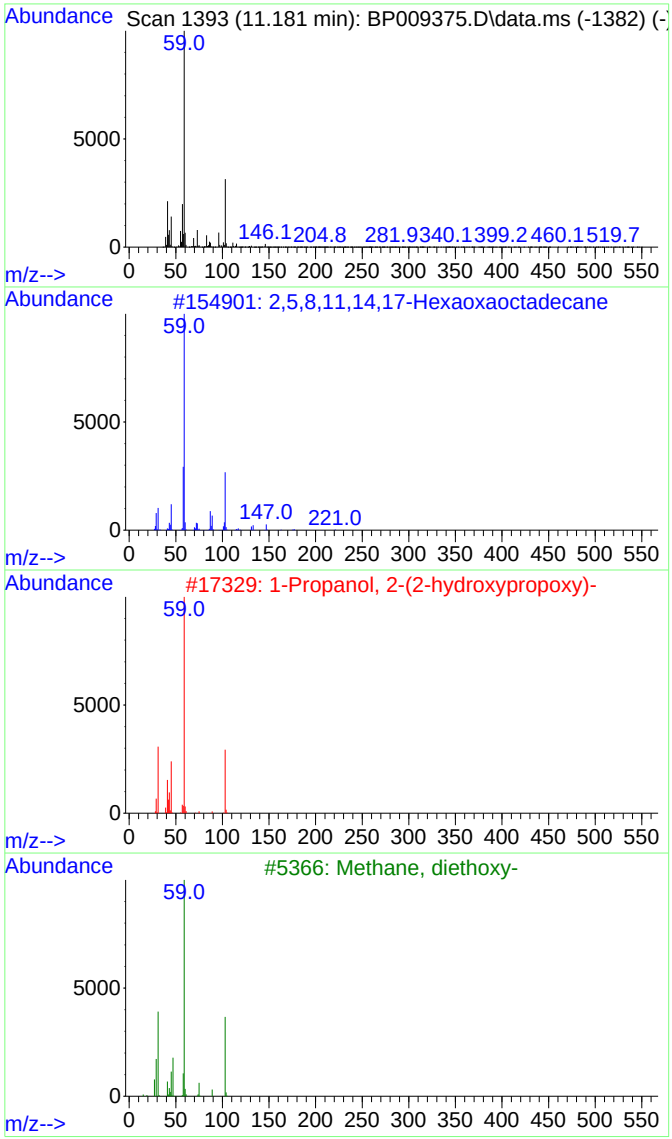
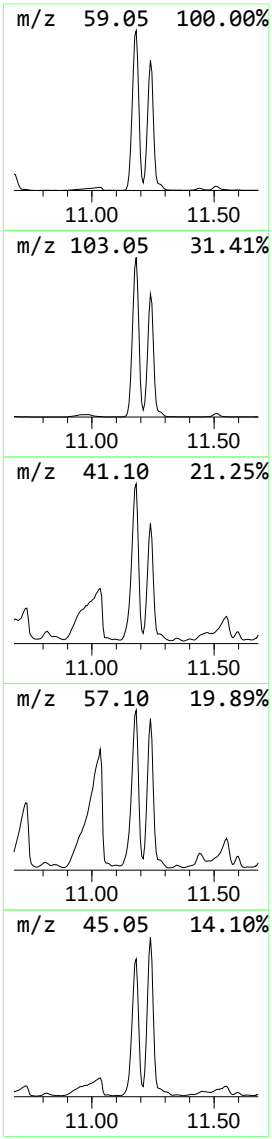
Peak Number 13 2,5,8,11,14,17-Hexaoxaoctad... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.181	118.97 ng	18739600	Naphthalene-d8	10.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5,8,11,14,17-Hexaoxaoctadecane	266	C12H26O6	001191-87-3	78
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
3	Methane, diethoxy-	104	C5H12O2	000462-95-3	72
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	72
5	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64





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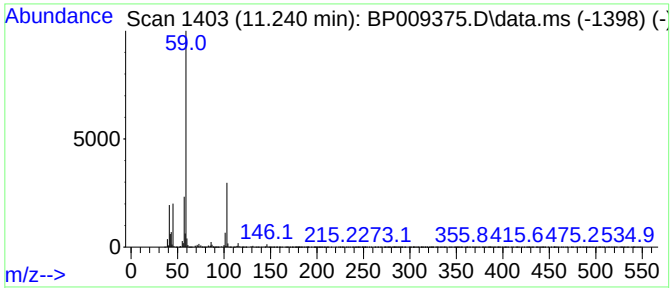
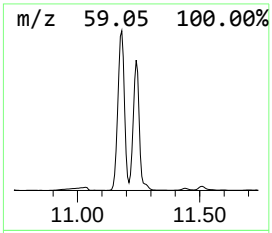
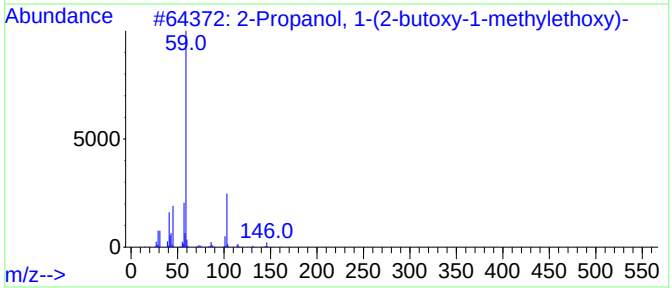
****
Peak Number 14 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 3

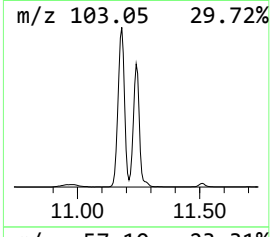
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.240	74.31 ng	11704800	Naphthalene-d8	10.610

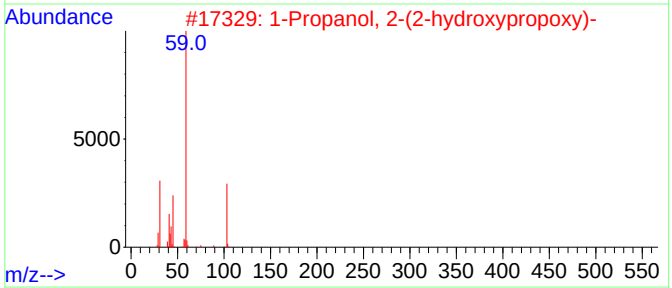
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	90
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78
3	Methane, diethoxy-	104	C5H12O2	000462-95-3	78
4	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	64

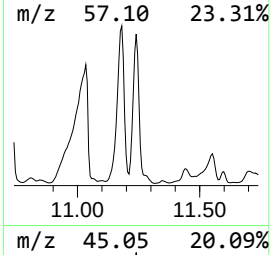


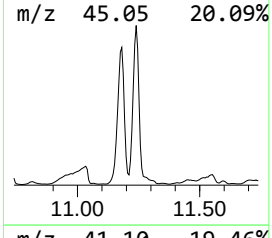


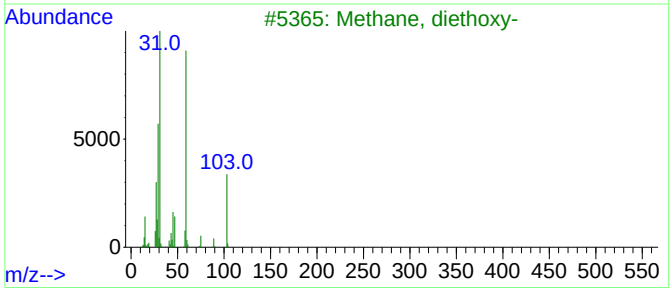


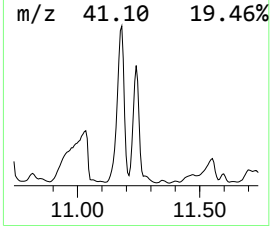












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031122\
Data File : BP009375.D
Acq On : 11 Mar 2022 20:54
Operator : CG/JU
Sample : N1886-03 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
30969

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

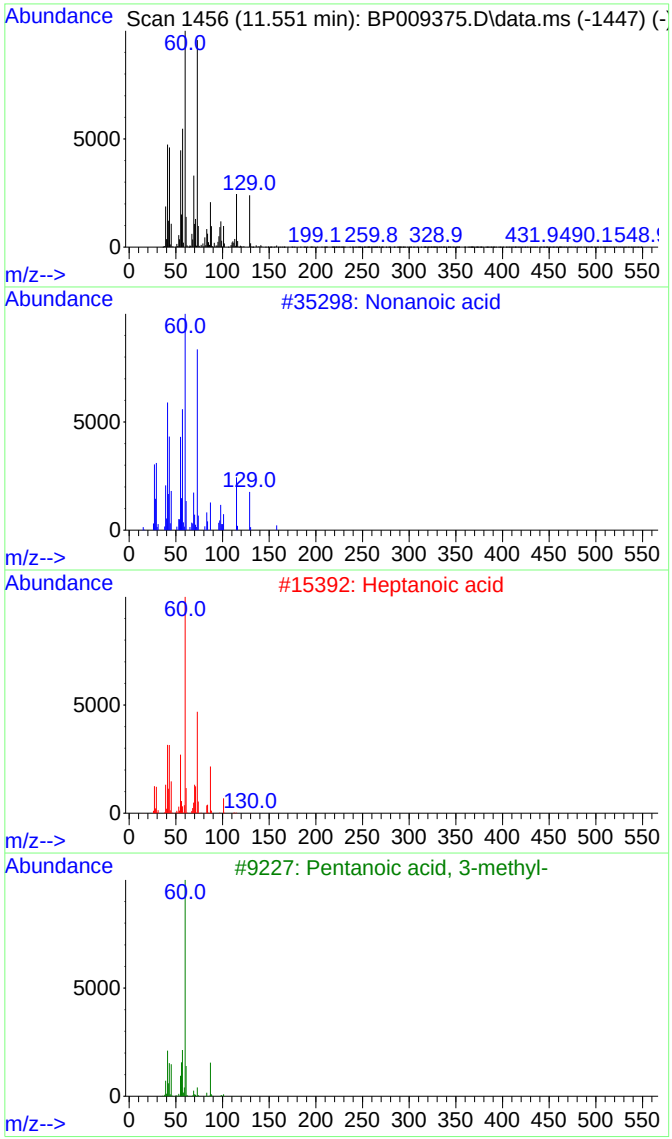
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

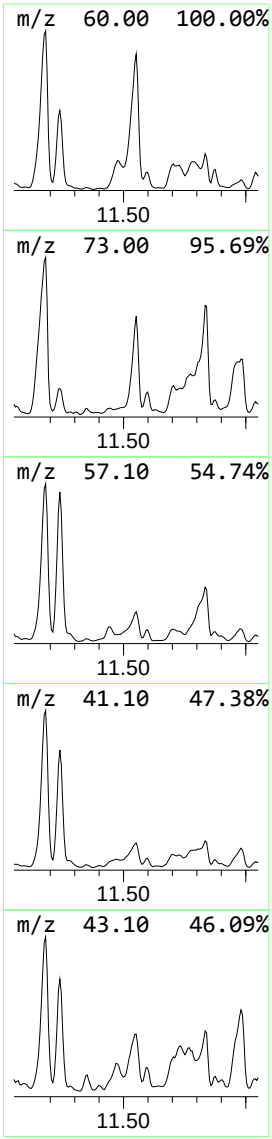
****

Peak Number 15 Nonanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.552	26.02 ng	4097720	Naphthalene-d8	10.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	87
2	Heptanoic acid	130	C7H14O2	000111-14-8	50
3	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	43
4	5-Methyloctanoic acid	158	C9H18O2	060218-42-0	42
5	D-Allose	180	C6H12O6	002595-97-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031122\
Data File : BP009375.D
Acq On : 11 Mar 2022 20:54
Operator : CG/JU
Sample : N1886-03 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
30969

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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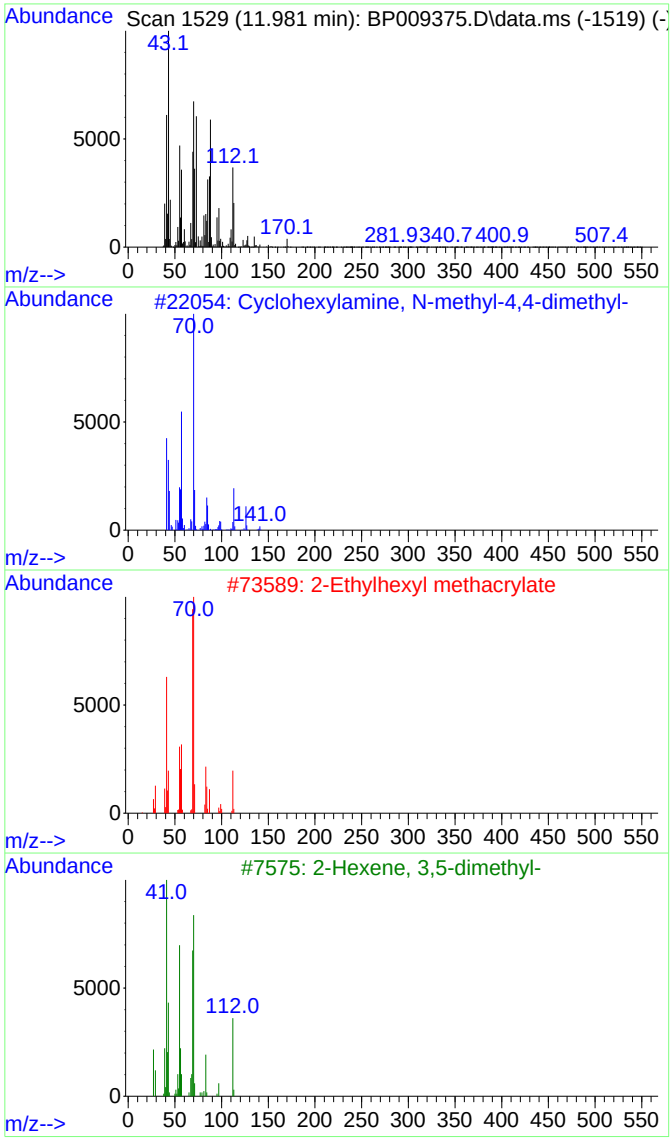
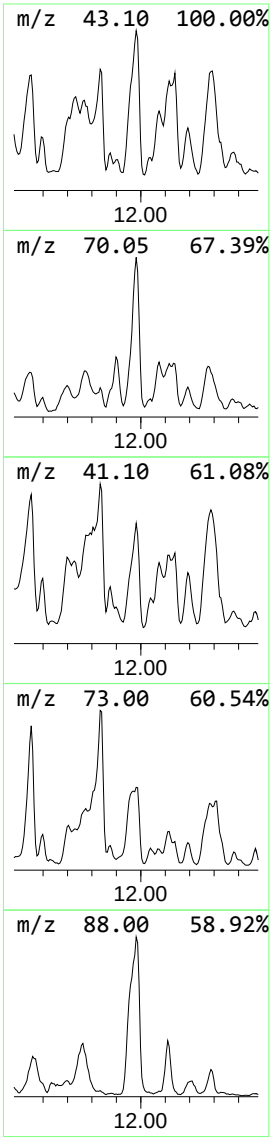
Peak Number 16 unknown11.981 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.981	19.72 ng	3106230	Naphthalene-d8	10.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexylamine, N-methyl-4,4-di...	141	C9H19N	045815-91-6	25
2	2-Ethylhexyl methacrylate	198	C12H22O2	000688-84-6	22
3	2-Hexene, 3,5-dimethyl-	112	C8H16	003404-79-3	22
4	Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	18
5	Hexane, 2-methyl-4-methylene-	112	C8H16	003404-80-6	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031122\
Data File : BP009375.D
Acq On : 11 Mar 2022 20:54
Operator : CG/JU
Sample : N1886-03 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
30969

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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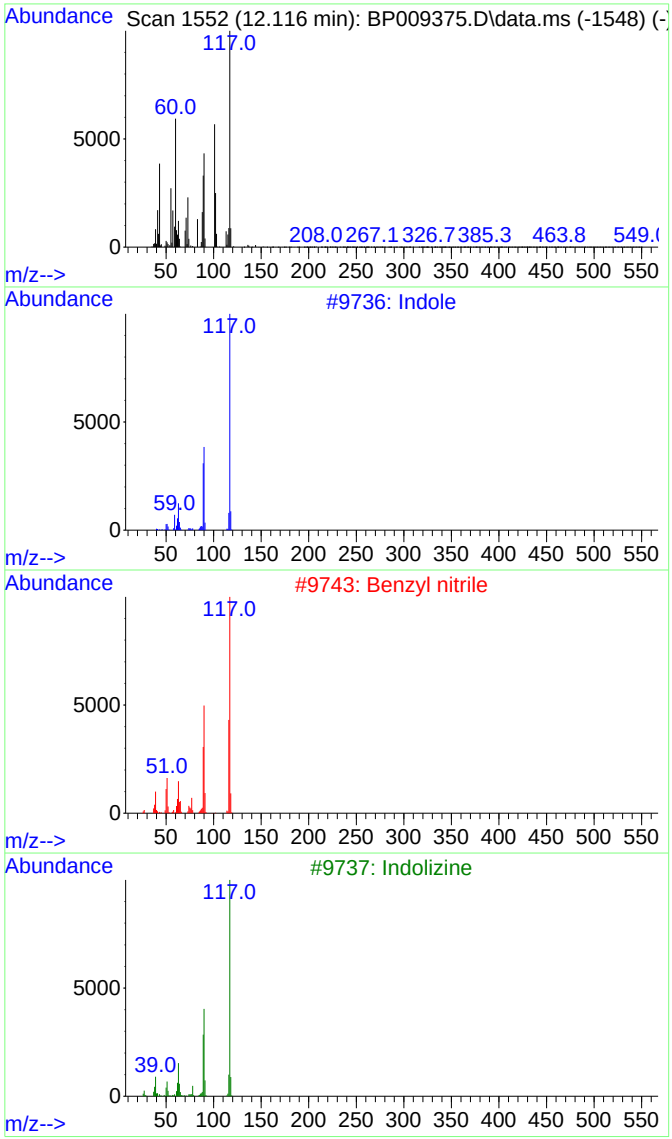
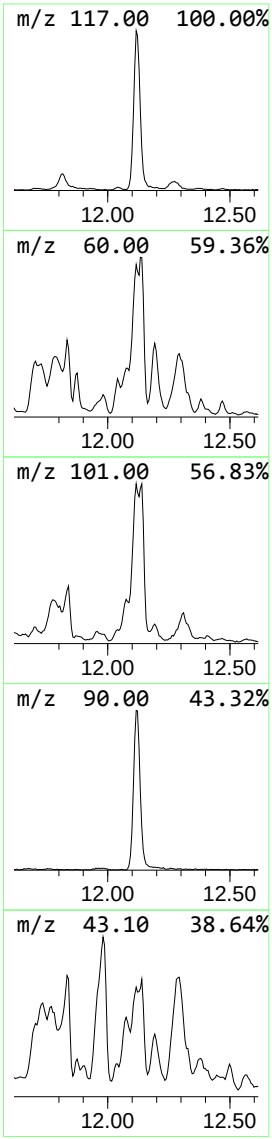
Peak Number 17 Indole Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.116	19.99 ng	3148400	Naphthalene-d8	10.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indole	117	C8H7N	000120-72-9	87
2	Benzyl nitrile	117	C8H7N	000140-29-4	50
3	Indolizine	117	C8H7N	000274-40-8	43
4	4-Ethynylaniline	117	C8H7N	014235-81-5	38
5	Benzonitrile, 2-methyl-	117	C8H7N	000529-19-1	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031122\
Data File : BP009375.D
Acq On : 11 Mar 2022 20:54
Operator : CG/JU
Sample : N1886-03 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
30969

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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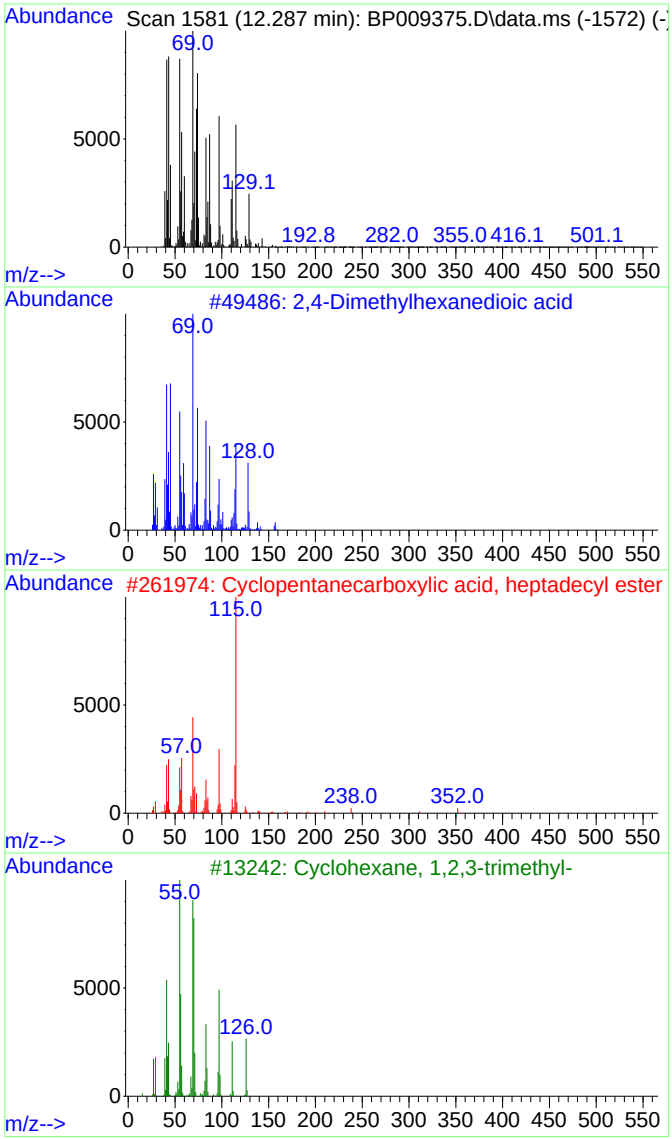
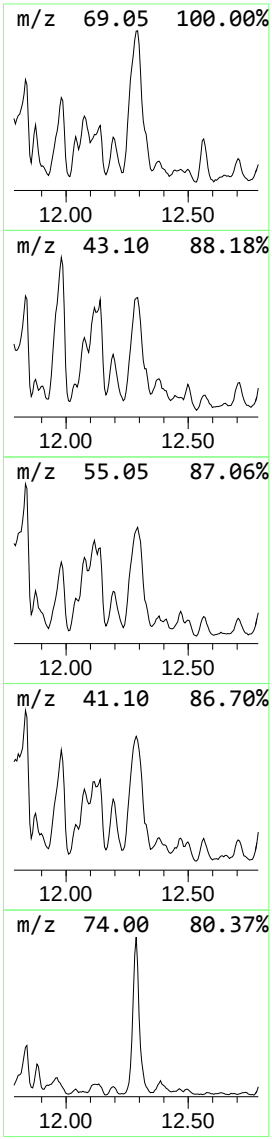
Peak Number 18 2,4-Dimethylhexanedioic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.287	29.50 ng	4646430	Naphthalene-d8	10.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dimethylhexanedioic acid	174	C8H14O4	040933-45-7	59
2	Cyclopentanecarboxylic acid, hep...	352	C23H44O2	1000282-77-6	27
3	Cyclohexane, 1,2,3-trimethyl-	126	C9H18	001678-97-3	27
4	Methyl 2-hydroxydecanoate	202	C11H22O3	071271-24-4	22
5	Cyclopropanecarboxylic acid, und...	240	C15H28O2	103677-78-7	22





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Data File : BP009375.D
Acq On : 11 Mar 2022 20:54
Operator : CG/JU
Sample : N1886-03 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
30969

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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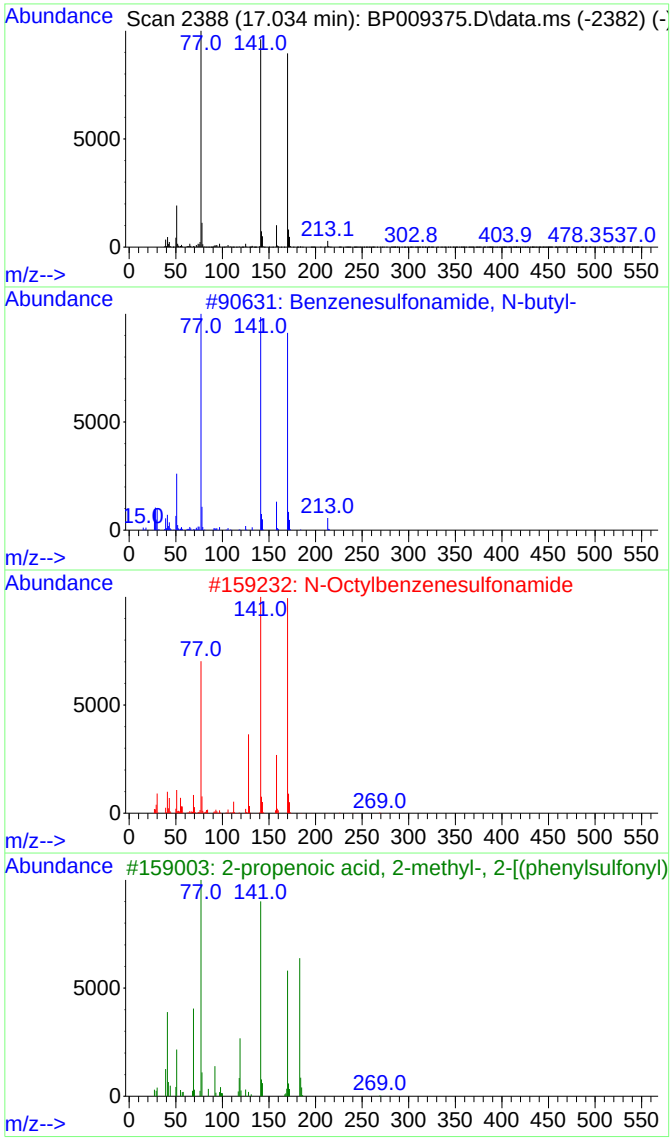
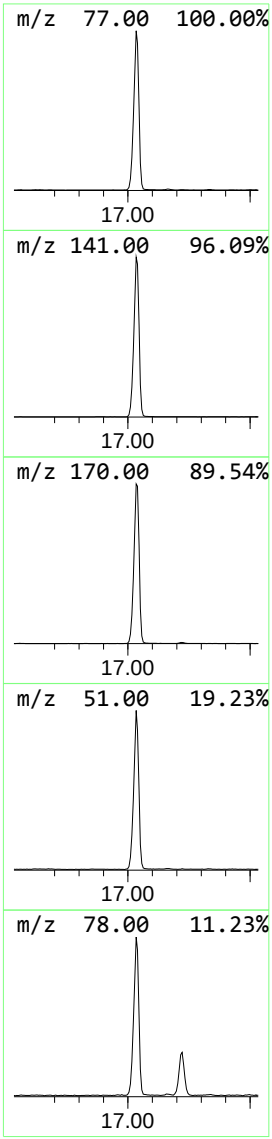
Peak Number 19 Benzenesulfonamide, N-butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.034	33.51 ng	7802430	Phenanthrene-d10	17.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N-butyl-	213	C10H15NO2S	003622-84-2	96
2	N-Octylbenzenesulfonamide	269	C14H23NO2S	016358-32-0	64
3	2-propenoic acid, 2-methyl-, 2-[...	269	C12H15NO4S	1000401-71-8	64
4	N-Benzenesulfonyloxy-2,2-bis(tri...	335	C10H7F6NO3S	055734-41-3	50
5	(Phenylsulfonyl)acetonitrile	181	C8H7NO2S	007605-28-9	47





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Data File : BP009375.D
Acq On : 11 Mar 2022 20:54
Operator : CG/JU
Sample : N1886-03 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
30969

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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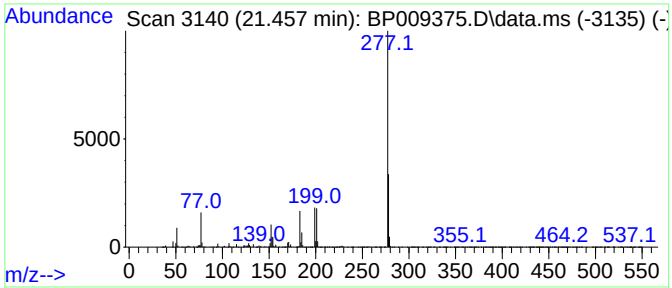
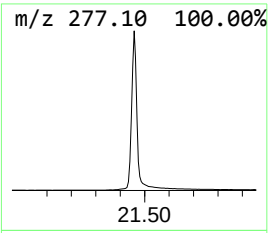
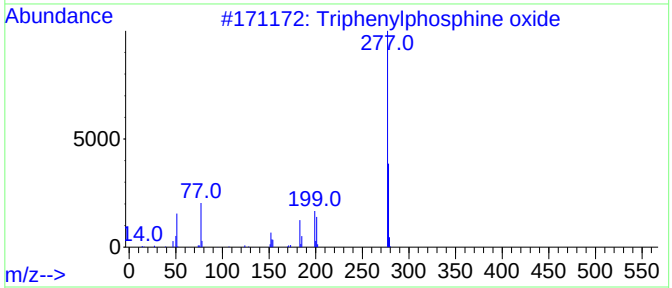
Peak Number 20 Triphenylphosphine oxide Concentration Rank 4

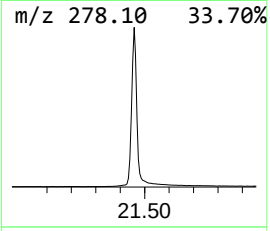
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.457	66.20 ng	17524400	Chrysene-d12	21.333

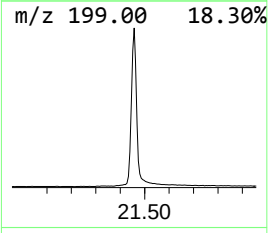
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	47
4	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	38
5	Oxoprophines	277	C17H11NO3	1000128-51-1	9

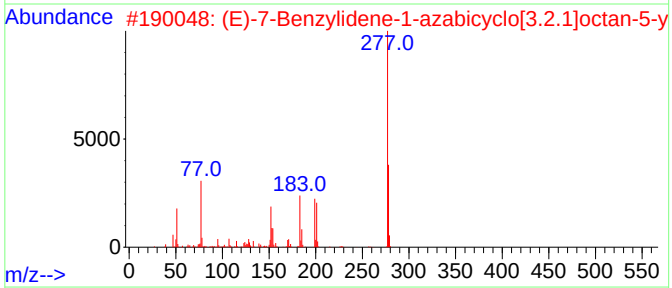


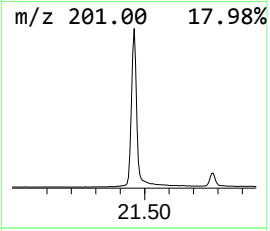


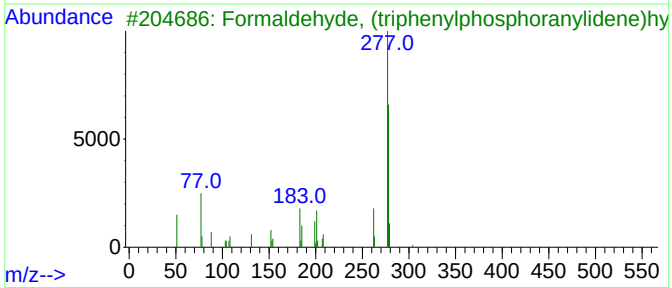


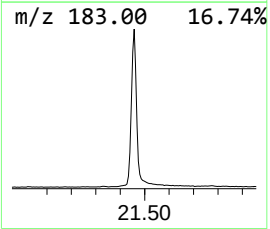












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031122\
Data File : BP009375.D
Acq On : 11 Mar 2022 20:54
Operator : CG/JU
Sample : N1886-03 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butanoic acid	4.087	28.3	ng	3051810	1	7.816	2159380	20.0
2-Furanmethanol	5.111	34.8	ng	3752150	1	7.816	2159380	20.0
1-Hexanol, 2-et...	7.899	14.2	ng	1530820	1	7.816	2159380	20.0
1-Butanol, 2-et...	9.052	17.7	ng	1909210	1	7.816	2159380	20.0
Hexanoic acid, ...	9.246	29.2	ng	4603470	2	10.610	3150220	20.0
2-Hexene, 3-met...	9.316	15.5	ng	2434480	2	10.610	3150220	20.0
3,3-Dimethylhep...	9.557	14.0	ng	2205900	2	10.610	3150220	20.0
Octanoic acid	10.105	24.2	ng	3808670	2	10.610	3150220	20.0
unknown10.557	10.557	14.4	ng	2269320	2	10.610	3150220	20.0
.alpha.-Terpineol	10.687	34.3	ng	5405460	2	10.610	3150220	20.0
3-Ethylheptanoi...	10.734	21.0	ng	3307530	2	10.610	3150220	20.0
4-Methyloctanoi...	11.034	104.0	ng	16374600	2	10.610	3150220	20.0
2,5,8,11,14,17-...	11.181	119.0	ng	18739600	2	10.610	3150220	20.0
2-Propanol, 1-(...	11.240	74.3	ng	11704800	2	10.610	3150220	20.0
Nonanoic acid	11.552	26.0	ng	4097720	2	10.610	3150220	20.0
unknown11.981	11.981	19.7	ng	3106230	2	10.610	3150220	20.0
Indole	12.116	20.0	ng	3148400	2	10.610	3150220	20.0
2,4-Dimethylhex...	12.287	29.5	ng	4646430	2	10.610	3150220	20.0
Benzenesulfonam...	17.034	33.5	ng	7802430	4	17.222	4656640	20.0
Triphenylphosph...	21.457	66.2	ng	17524400	5	21.333	5294680	20.0