LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060823\
Data File : BM040176.D
Acq On : 09 Jun 2023 02:57
Operator : MA/JU
Sample : 03046-07
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-2-6-10

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_M\Methods\8270-BM060823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM040176.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.381	11	16	31	rVB	3367651	4399685	11.44%	0.819%
2	3.652	54	62	66	rBV	352282	554274	1.44%	0.103%
3	3.816	88	90	99	rBV	820095	1176883	3.06%	0.219%
4	4.034	119	127	128	rBV2	322346	550614	1.43%	0.102%
5	4.105	134	139	142	rVB2	559317	1069792	2.78%	0.199%
6	4.499	198	206	214	rVB	377242	553478	1.44%	0.103%
7	4.587	214	221	231	rVB	303640	429740	1.12%	0.080%
8	4.828	255	262	267	rBV	340882	601884	1.57%	0.112%
9	4.981	276	288	291	rBV2	189843	414933	1.08%	0.077%
10	5.140	310	315	324	rVB	327468	475776	1.24%	0.089%
11	5.540	377	383	392	rVB	4221057	6016072	15.65%	1.119%
12	6.052	461	470	477	rBV	5112751	7449604	19.38%	1.386%
13	6.134	477	484	488	rVB	311250	431295	1.12%	0.080%
14	7.146	648	656	668	rVB	2470892	4136850	10.76%	0.770%
15	7.363	689	693	699	rVB	433929	636066	1.65%	0.118%
16	7.575	723	729	733	rBV	308853	475254	1.24%	0.088%
17	7.716	749	753	765	rVB	325741	600251	1.56%	0.112%
18	7.987	793	799	806	rBV	1577641	2409144	6.27%	0.448%
19	8.322	852	856	862	rVB	284926	450866	1.17%	0.084%
20	8.751	924	929	935	rBV3	235218	424541	1.10%	0.079%
21	8.816	935	940	945	rVB2	264568	434281	1.13%	0.081%
22	9.075	977	984	992	rBV	996893	1909238	4.97%	0.355%
23	9.157	992	998	1005	rVV	4537352	7498002	19.50%	1.395%
24	9.222	1005	1009	1019	rVB4	262135	526830	1.37%	0.098%
25	9.316	1019	1025	1031	rBV2	210359	389573	1.01%	0.072%
26	9.498	1046	1056	1061	rBV2	458146	999492	2.60%	0.186%
27	9.693	1082	1089	1097	rVB5	294643	932993	2.43%	0.174%
28	10.022	1138	1145	1151	rVB4	191285	457605	1.19%	0.085%
29	10.087	1151	1156	1163	rBV3	211912	459985	1.20%	0.086%
30	10.351	1195	1201	1210	rVB	654636	1179260	3.07%	0.219%
31	10.451	1211	1218	1228	rBV5	387948	1007754	2.62%	0.188%
32	10.798	1268	1277	1284	rBV	1877577	3841156	9.99%	0.715%
33	10.916	1291	1297	1303	rVB4	408354	882998	2.30%	0.164%
34	11.022	1306	1315	1324	rVB4	718256	1843356	4.79%	0.343%
35	11.157	1332	1338	1350	rVB	3041442	5683156	14.78%	1.057%
36	11.369	1370	1374	1381	rBV3	321895	630577	1.64%	0.117%

LSC Area Percent Report

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Data File : BM040176.D
Acq On : 09 Jun 2023 02:57
Operator : MA/JU
Sample : 03046-07
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-2-6-10

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_M\Methods\8270-BM060823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.451	1381	1388	1400	rVB5	407717	1685961	4.39%	0.314%
38	11.569	1401	1408	1409	rBV4	199609	398164	1.04%	0.074%
39	11.728	1426	1435	1440	rBV2	556365	1242916	3.23%	0.231%
40	11.798	1440	1447	1450	rBV3	375122	780042	2.03%	0.145%
41	11.945	1468	1472	1475	rBV2	309388	465366	1.21%	0.087%
42	12.034	1481	1487	1492	rBV	4434524	6601922	17.17%	1.228%
43	12.157	1499	1508	1513	rBV4	830083	1959144	5.10%	0.365%
44	12.216	1514	1518	1523	rVV2	499968	786001	2.04%	0.146%
45	12.269	1523	1527	1532	rVB2	734638	971829	2.53%	0.181%
46	12.322	1533	1536	1542	rVB2	414954	650914	1.69%	0.121%
47	12.392	1543	1548	1551	rBV	1682373	3125523	8.13%	0.582%
48	12.422	1551	1553	1560	rVB	1405537	2037313	5.30%	0.379%
49	12.492	1560	1565	1568	rBV2	707212	1221763	3.18%	0.227%
50	12.575	1572	1579	1585	rBV2	1295660	2644179	6.88%	0.492%
51	12.751	1605	1609	1611	rBV	1593345	2242444	5.83%	0.417%
52	12.781	1612	1614	1617	rVB	904001	1211944	3.15%	0.226%
53	12.945	1637	1642	1648	rBV4	2566417	5760958	14.99%	1.072%
54	12.998	1648	1651	1655	rBV2	1055246	1643248	4.27%	0.306%
55	13.051	1656	1660	1665	rVV2	4190047	6366069	16.56%	1.185%
56	13.151	1670	1677	1682	rBV4	2773862	6360904	16.55%	1.184%
57	13.204	1683	1686	1690	rBV3	1543917	2137677	5.56%	0.398%
58	13.257	1690	1695	1699	rBV	9972867	13701610	35.64%	2.549%
59	13.369	1710	1714	1718	rBV	2470936	4206366	10.94%	0.783%
60	13.498	1734	1736	1739	rBV	902319	936773	2.44%	0.174%
61	13.533	1739	1742	1745	rVB	1733558	1972060	5.13%	0.367%
62	13.581	1746	1750	1754	rBV	3156555	4598521	11.96%	0.856%
63	13.680	1760	1767	1774	rVB2	9603933	25487611	66.30%	4.742%
64	13.745	1774	1778	1780	rBV	1793283	2508085	6.52%	0.467%
65	13.780	1780	1784	1788	rVB3	2587106	4559117	11.86%	0.848%
66	13.880	1798	1801	1804	rVB	1858249	1999444	5.20%	0.372%
67	13.922	1805	1808	1812	rBV	1440498	2143722	5.58%	0.399%
68	14.004	1818	1822	1827	rBV2	1583160	2422883	6.30%	0.451%
69	14.092	1834	1837	1841	rVB2	1306402	1600074	4.16%	0.298%
70	14.151	1844	1847	1850	rBV4	1277319	2064551	5.37%	0.384%
71	14.269	1863	1867	1871	rBV2	1395142	2780648	7.23%	0.517%
72	14.357	1880	1882	1885	rBV2	850418	875630	2.28%	0.163%
73	14.510	1905	1908	1914	rBV4	1003703	2211909	5.75%	0.412%
74	14.575	1915	1919	1923	rBV	5825344	8229905	21.41%	1.531%
75	14.627	1924	1928	1930	rVV	2502644	3524001	9.17%	0.656%
76	14.657	1931	1933	1936	rVB	1611195	1772176	4.61%	0.330%

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Integration Parameters: rteint.p
Integrator: RTE
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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	14.792	1953	1956	1960	rVB	4683027	5805843	15.10%	1.080%
78	14.845	1961	1965	1968	rVB4	1838813	2649764	6.89%	0.493%
79	15.010	1991	1993	1996	rBV2	1471668	1735523	4.51%	0.323%
80	15.445	2064	2067	2070	rBV	2203542	3236156	8.42%	0.602%
81	15.563	2083	2087	2092	rBV2	7190713	10724116	27.90%	1.995%
82	15.663	2101	2104	2107	rBV2	3863695	4908438	12.77%	0.913%
83	15.816	2127	2130	2137	rBV2	2581367	4901043	12.75%	0.912%
84	16.116	2178	2181	2186	rVB2	5983994	8105394	21.08%	1.508%
85	16.304	2210	2213	2216	rVB	4170061	4791180	12.46%	0.891%
86	16.457	2235	2239	2242	rBV	5182374	6759154	17.58%	1.258%
87	16.610	2262	2265	2269	rVV	8548677	10990317	28.59%	2.045%
88	16.651	2269	2272	2276	rVB	9451837	11657791	30.32%	2.169%
89	16.763	2287	2291	2297	rVB2	15313266	23495332	61.12%	4.372%
90	16.833	2300	2303	2306	rVB	3714292	4593292	11.95%	0.855%
91	16.963	2321	2325	2329	rBV	12659740	16869946	43.88%	3.139%
92	17.286	2373	2380	2387	rBV3	16895456	38443951	100.00%	7.153%
93	17.380	2391	2396	2397	rBV2	16704246	25953529	67.51%	4.829%
94	17.445	2401	2407	2414	rBV2	16816654	32839948	85.42%	6.111%
95	17.551	2420	2425	2429	rVB	15310294	27413542	71.31%	5.101%
96	17.751	2453	2459	2463	rBV	13905115	30397695	79.07%	5.656%
97	17.786	2463	2465	2469	rVB	6750286	6821541	17.74%	1.269%
98	18.039	2504	2508	2510	rBV2	12727286	20861891	54.27%	3.882%
99	18.104	2515	2519	2521	rBV	5283256	8867741	23.07%	1.650%
100	18.180	2527	2532	2540	rVB	10674530	24788367	64.48%	4.612%

Sum of corrected areas: 537434119

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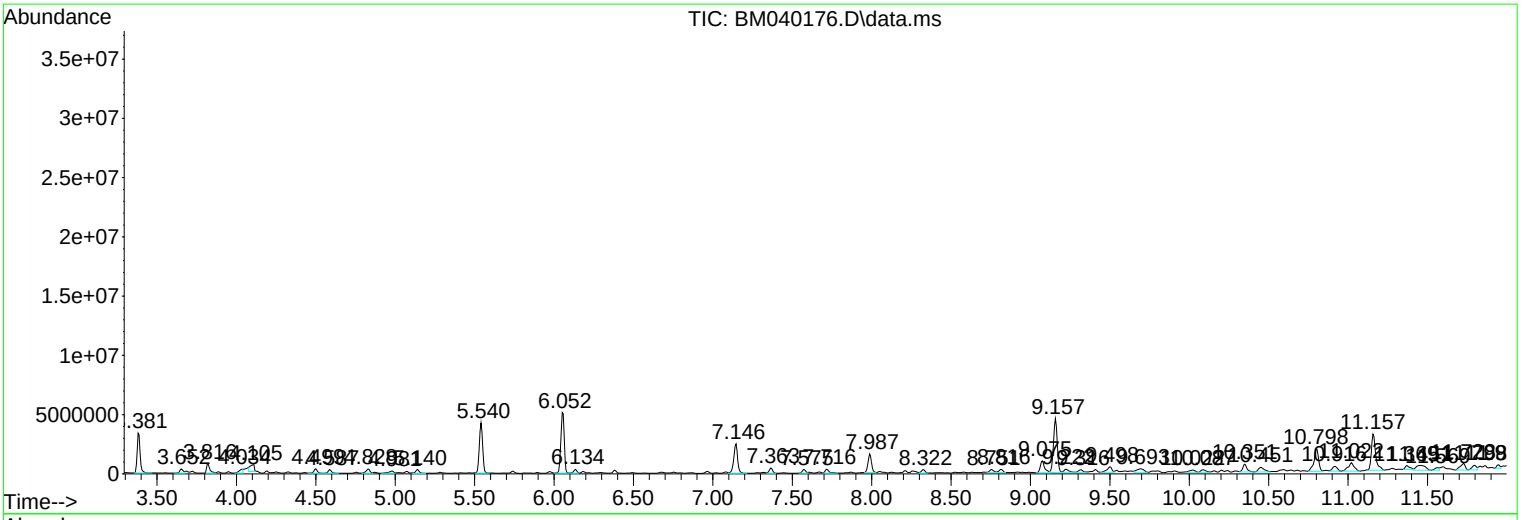
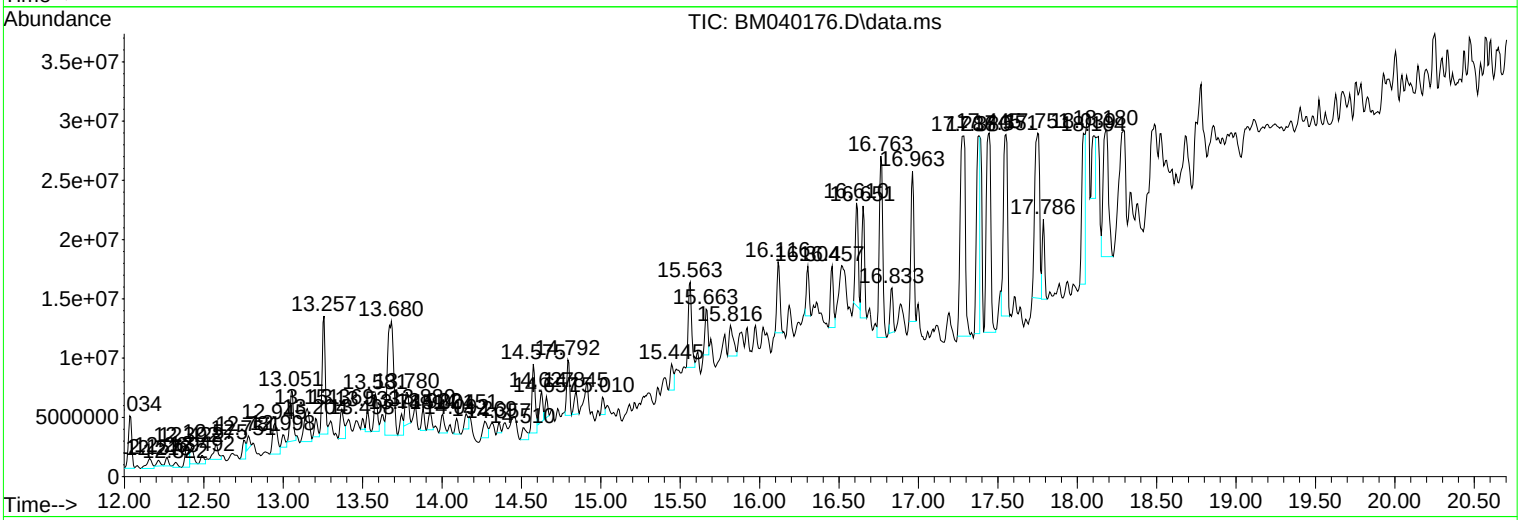
ALS Vial : 27 Sample Multiplier: 1

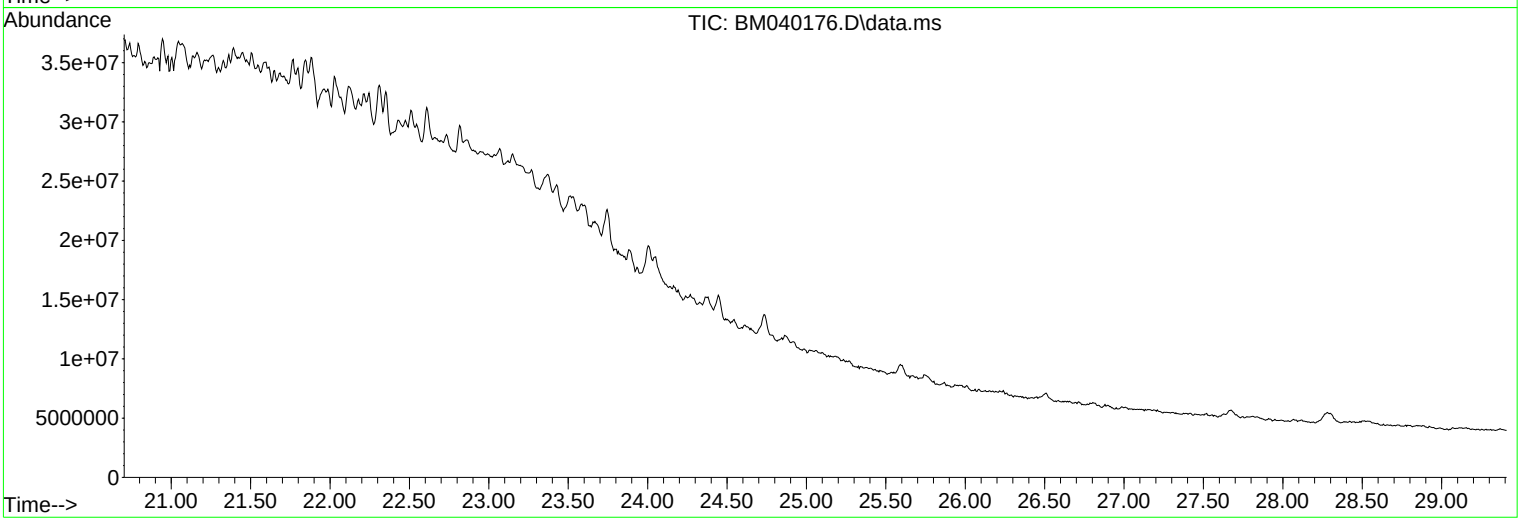
Instrument :
BNA_M
ClientSampleId :
COMP-2-6-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060823.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_M\Data\BM060823\
Data File : BM040176.D
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

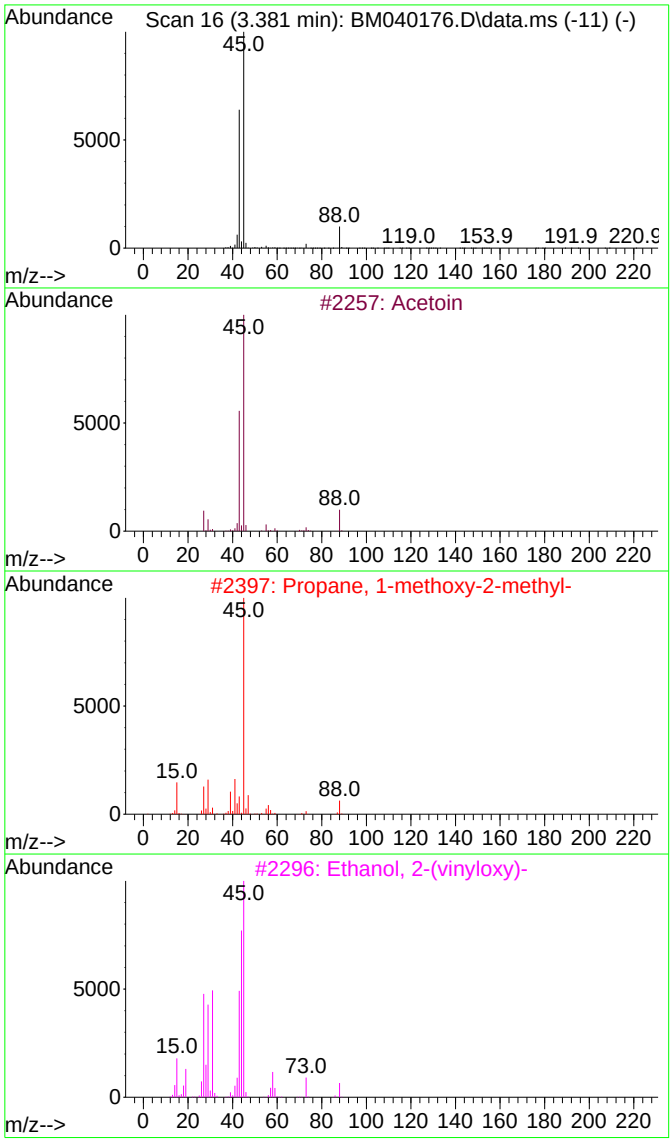
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

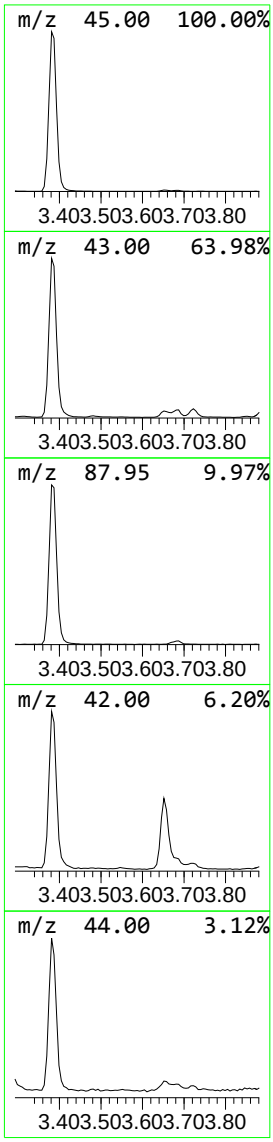
****

Peak Number 1 Acetoin Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.381	36.52 ng	4399690	1,4-Dichlorobenzene-d4	7.987

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetoin	88	C4H8O2	000513-86-0	90
2	Propane, 1-methoxy-2-methyl-	88	C5H12O	000625-44-5	56
3	Ethanol, 2-(vinyloxy)-	88	C4H8O2	000764-48-7	9
4	Isoamyl lactate	160	C8H16O3	019329-89-6	9
5	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	7





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

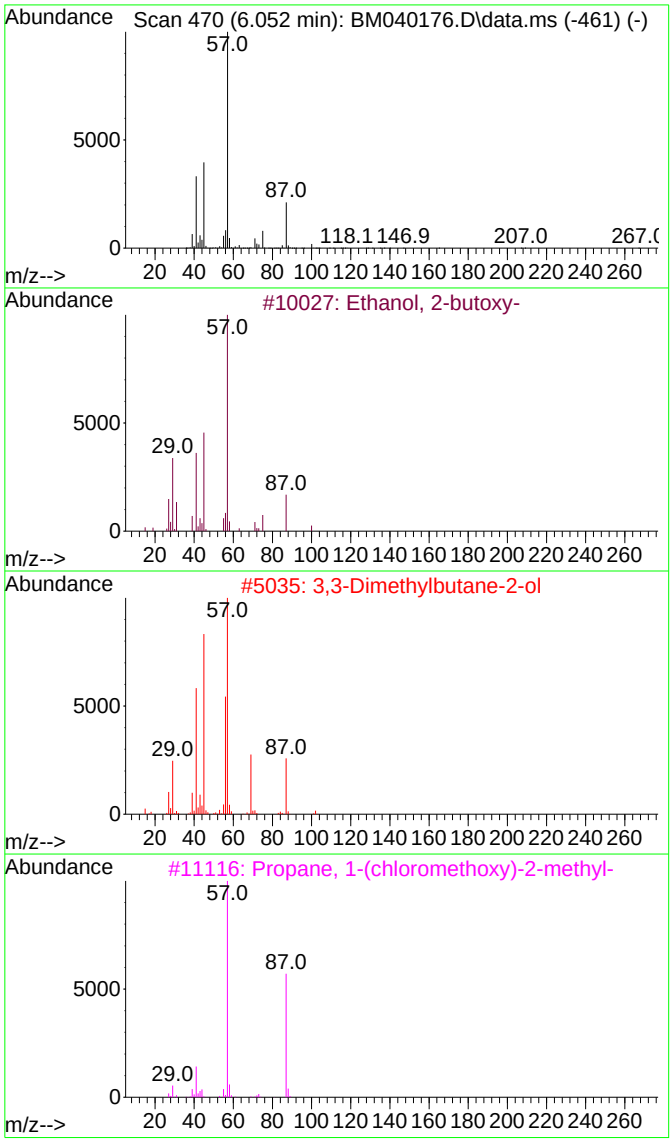
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

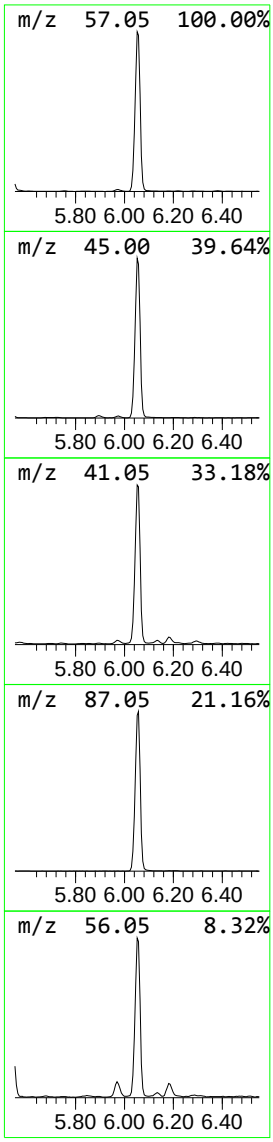
****

Peak Number 2 Ethanol, 2-butoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.052	61.84 ng	7449600	1,4-Dichlorobenzene-d4	7.987

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
2	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	59
3	Propane, 1-(chloromethoxy)-2-met...	122	C5H11ClO	034180-11-5	35
4	Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	35
5	Formic acid, 3,3-dimethylbut-2-y...	130	C7H14O2	1000368-20-5	25





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060823.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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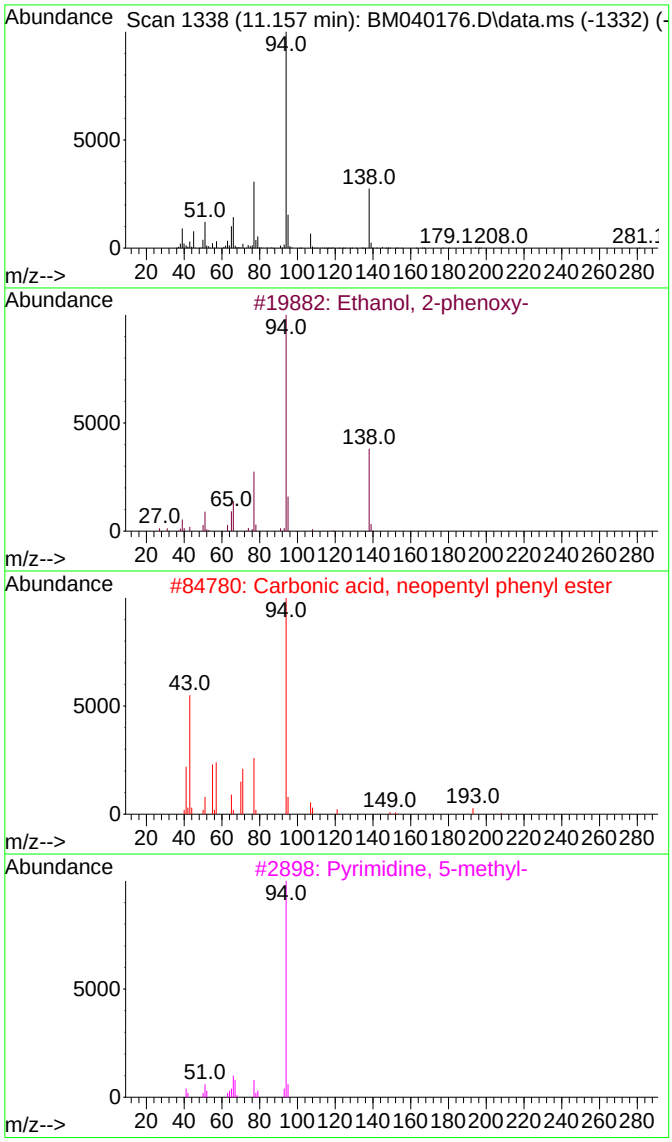
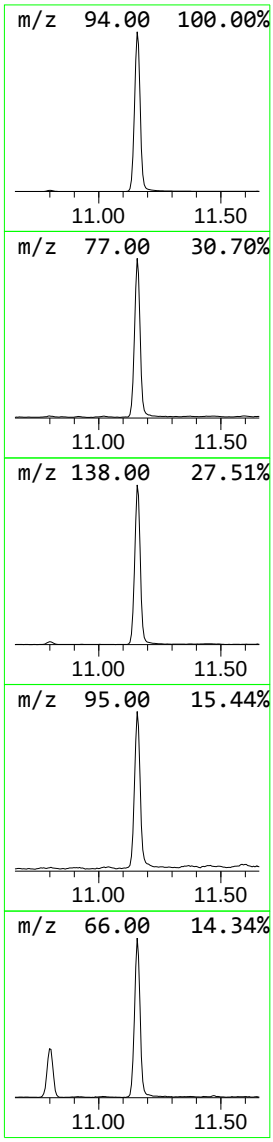
Peak Number 3 Ethanol, 2-phenoxy- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.157	29.59 ng	5683160	Naphthalene-d8	10.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	94
2	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
3	Pyrimidine, 5-methyl-	94	C5H6N2	002036-41-1	53
4	Acetic acid, phenyl ester	136	C8H8O2	000122-79-2	50
5	Phenol	94	C6H6O	000108-95-2	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060823\
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060823.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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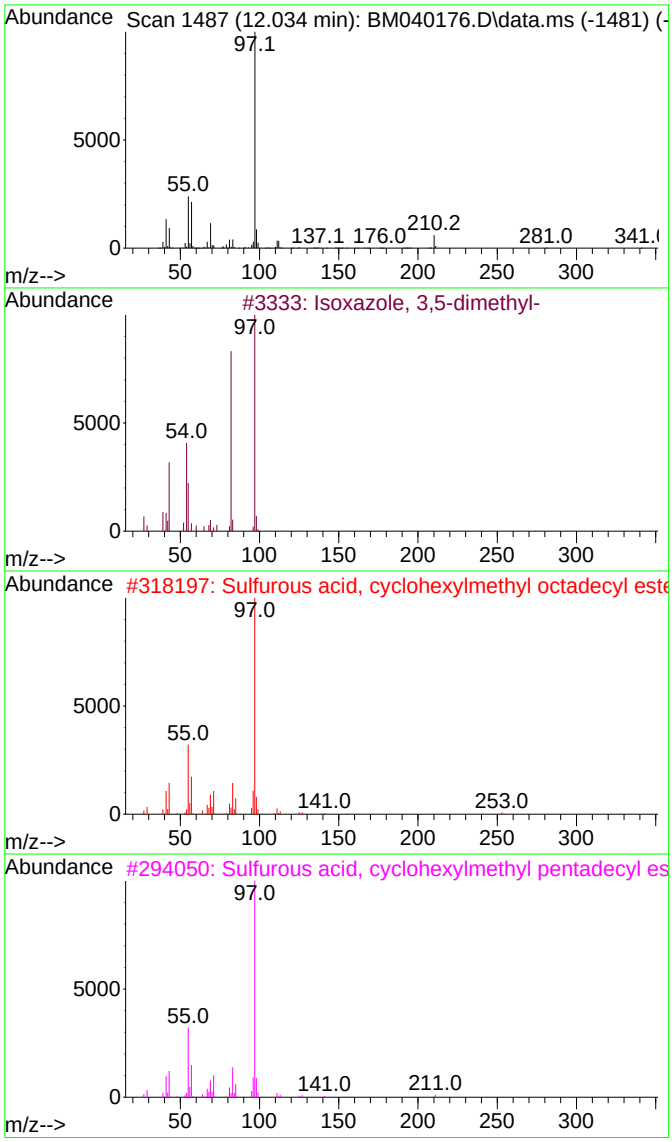
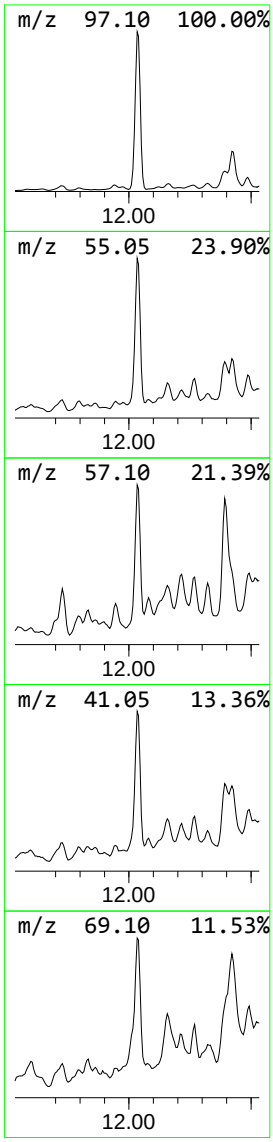
Peak Number 4 Isoxazole, 3,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.034	34.37 ng	6601920	Naphthalene-d8	10.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	64
2	Sulfurous acid, cyclohexylmethyl...	430	C25H50O3S	1000309-22-6	50
3	Sulfurous acid, cyclohexylmethyl...	388	C22H44O3S	1000309-22-3	50
4	1-(Trimethylsilyl)-1-propyne	112	C6H12Si	006224-91-5	39
5	Sulfurous acid, cyclohexylmethyl...	374	C21H42O3S	1000309-22-2	39





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060823\
Data File : BM040176.D
Acq On : 09 Jun 2023 02:57
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ALS Vial : 27 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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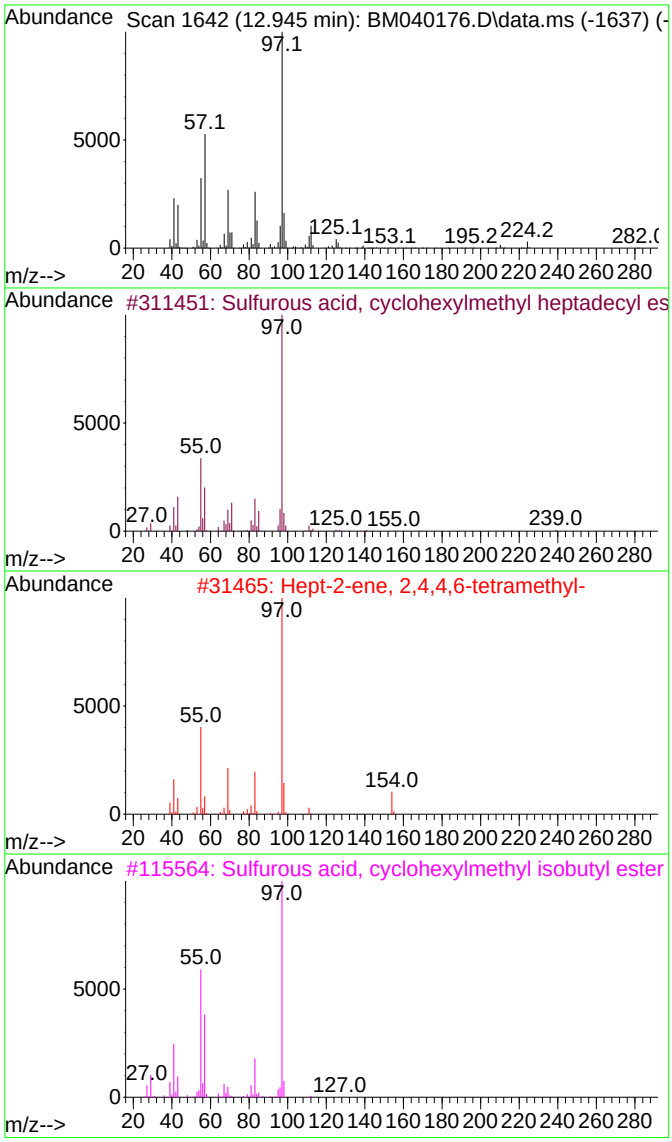
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

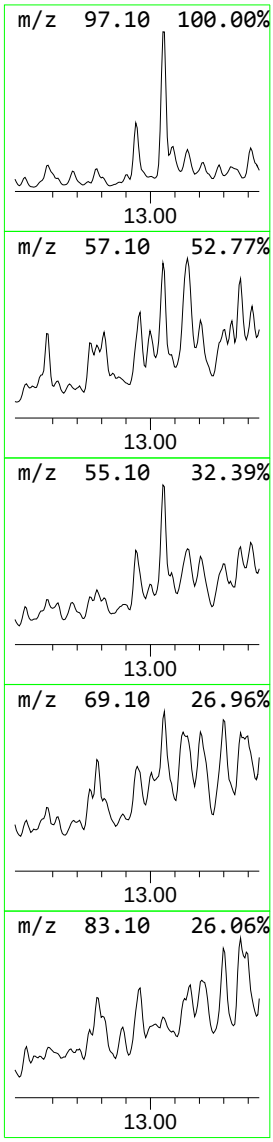
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Sulfurous acid, cyclohexylm... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.945	32.70 ng	5760960	Acenaphthene-d10	14.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, cyclohexylmethyl...	416	C24H48O3S	1000309-22-5	59
2	Hept-2-ene, 2,4,4,6-tetramethyl-	154	C11H22	103982-58-7	59
3	Sulfurous acid, cyclohexylmethyl...	234	C11H22O3S	1000309-21-3	53
4	1-(Trimethylsilyl)-1-propyne	112	C6H12Si	006224-91-5	53
5	Sulfurous acid, cyclohexylmethyl...	360	C20H40O3S	1000309-22-1	53





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Acq On : 09 Jun 2023 02:57
Operator : MA/JU
Sample : 03046-07
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-2-6-10

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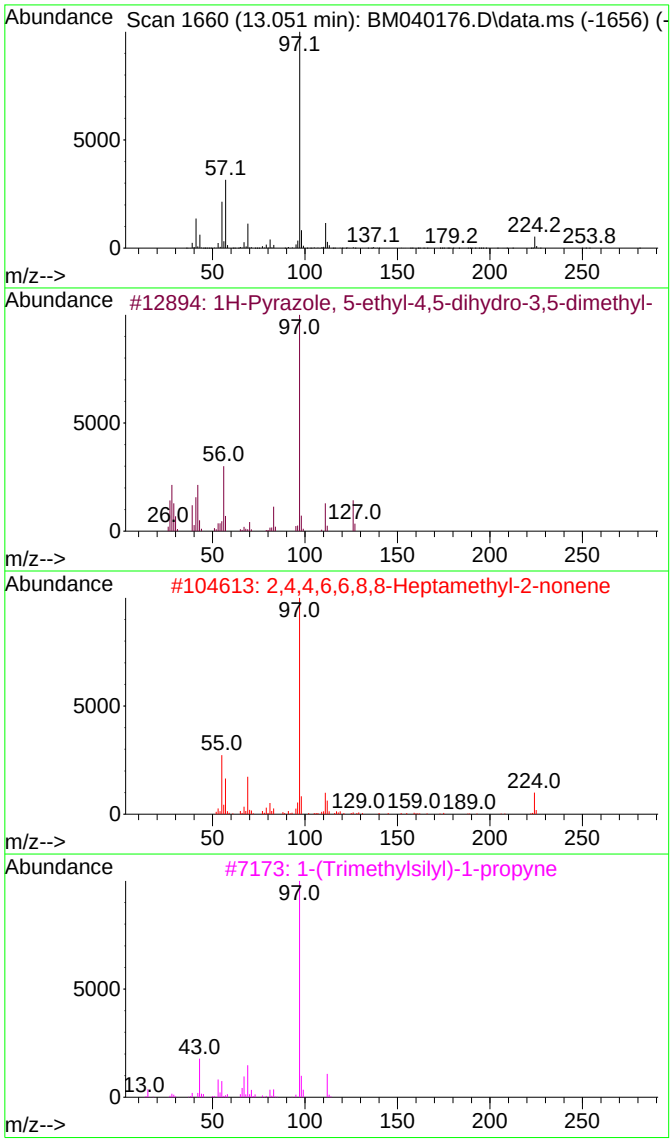
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

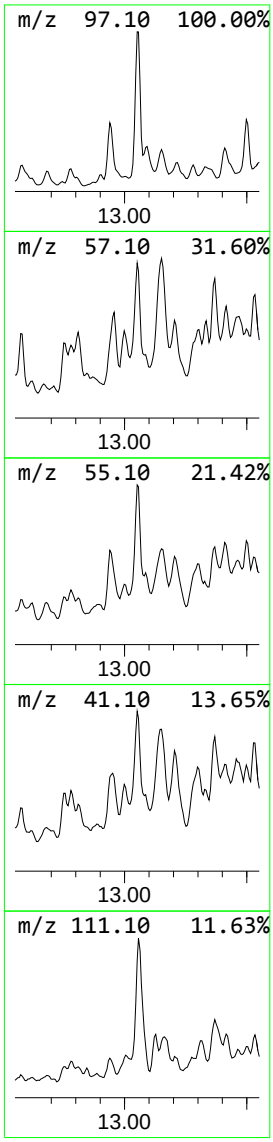
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1H-Pyrazole, 5-ethyl-4,5-di... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.051	36.13 ng	6366070	Acenaphthene-d10	14.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole, 5-ethyl-4,5-dihydro...	126	C7H14N2	021981-22-6	72
2	2,4,4,6,6,8,8-Heptamethyl-2-nonene	224	C16H32	039761-73-4	46
3	1-(Trimethylsilyl)-1-propyne	112	C6H12Si	006224-91-5	39
4	Sulfurous acid, cyclohexylmethyl...	374	C21H42O3S	1000309-22-2	39
5	2H-Pyran-4-carboxylic acid, 3,4-...	170	C9H14O3	038858-64-9	39





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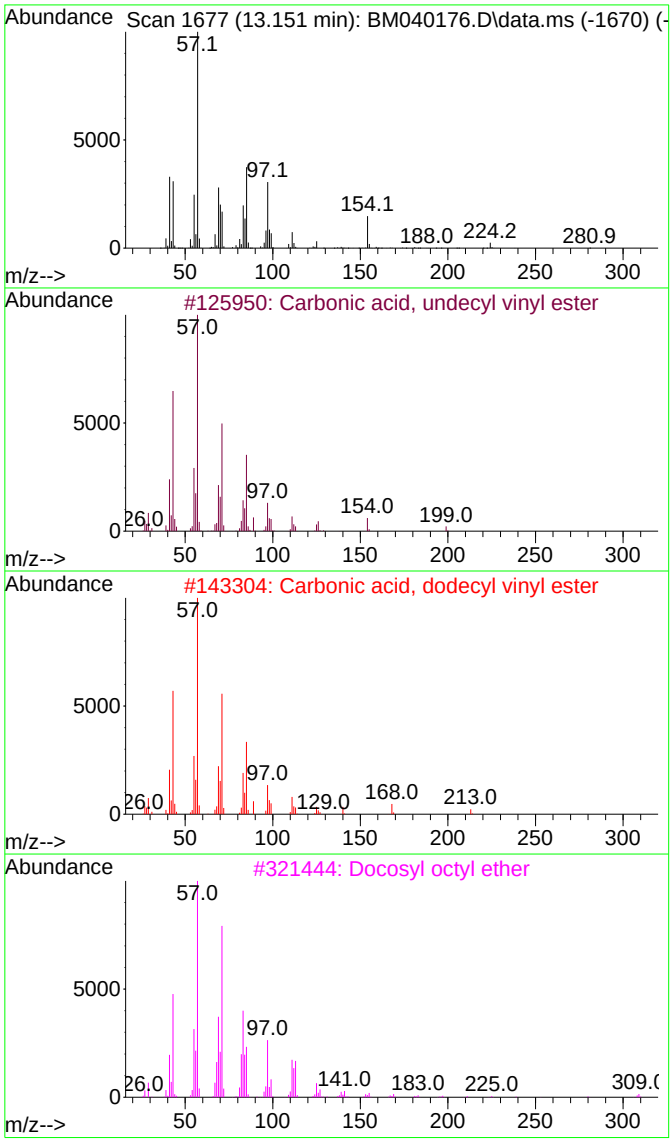
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

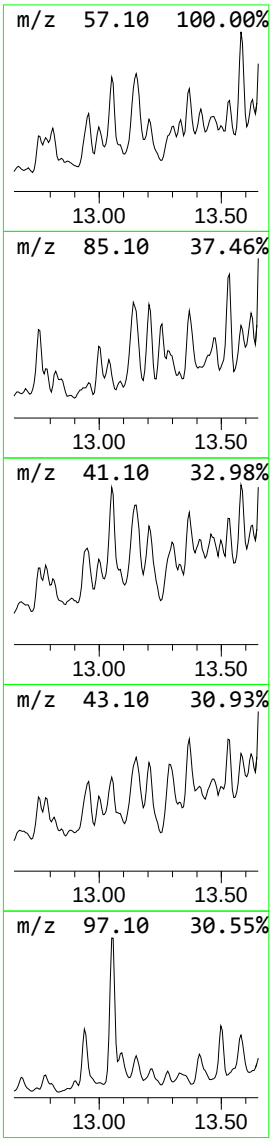
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Carbonic acid, undecyl viny... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.151	36.10 ng	6360900	Acenaphthene-d10	14.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, undecyl vinyl ester	242	C14H26O3	1000382-54-9	72
2	Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	64
3	Docosyl octyl ether	438	C30H62O	1000406-38-9	53
4	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	50
5	Isobutyl undecyl carbonate	272	C16H32O3	1000372-78-8	47





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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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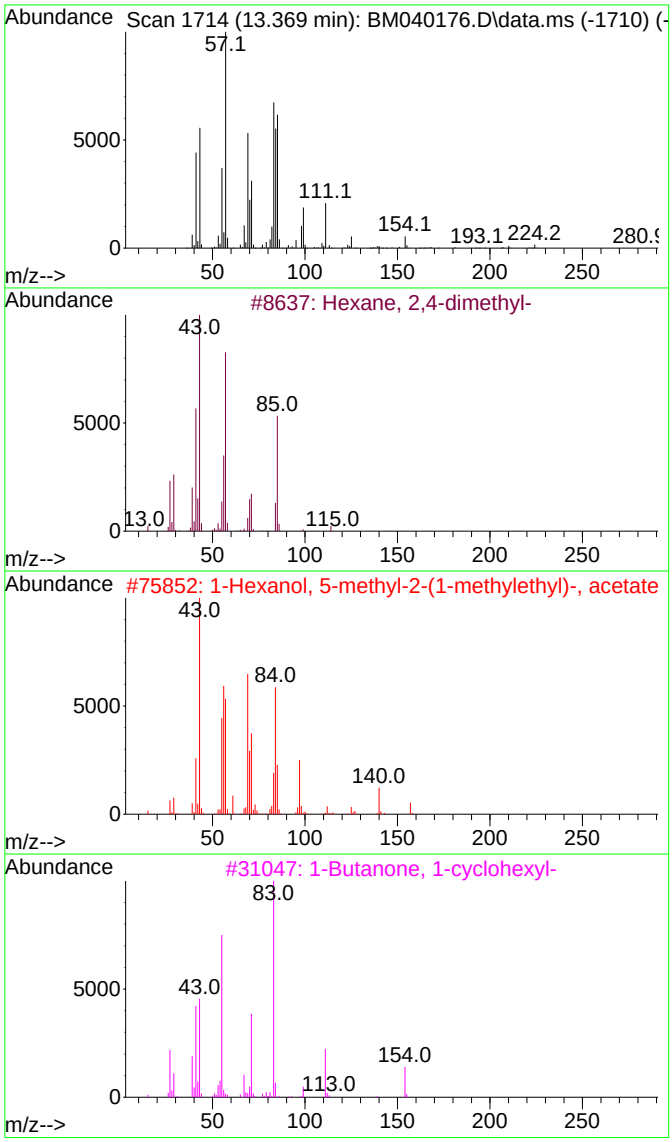
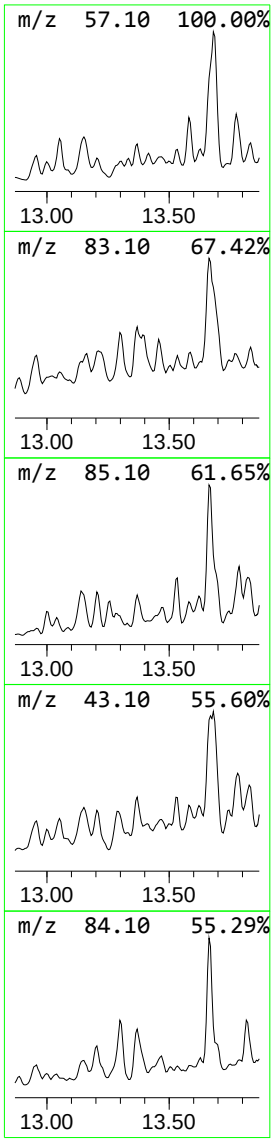
Peak Number 8 unknown13.369 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.369	23.87 ng	4206370	Acenaphthene-d10	14.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	38
2	1-Hexanol, 5-methyl-2-(1-methyle...	200	C12H24O2	040853-55-2	35
3	1-Butanone, 1-cyclohexyl-	154	C10H18O	001462-27-7	27
4	Heptane, 2,2,3,3,5,6,6-heptamethyl-	198	C14H30	007225-67-4	27
5	Butanoic acid, 2-methyl-, 1,2-di...	172	C10H20O2	084696-83-3	22





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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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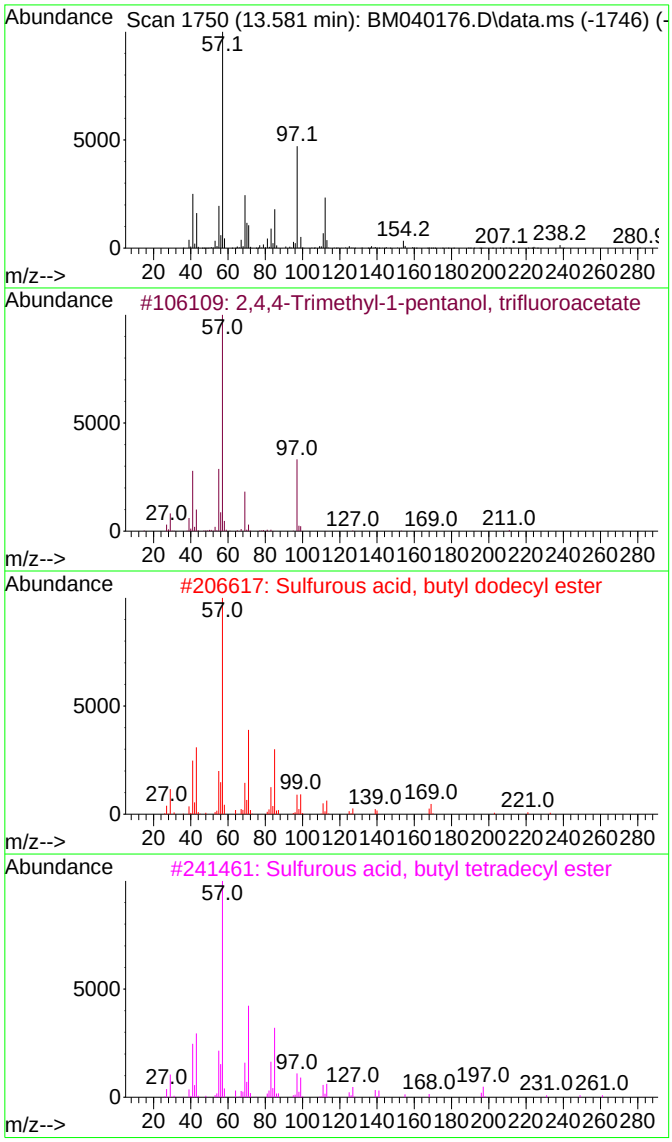
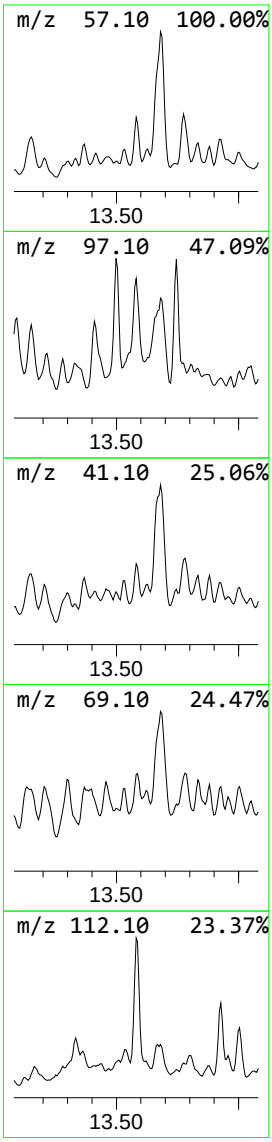
Peak Number 9 unknown13.581 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.581	26.10 ng	4598520	Acenaphthene-d10	14.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	43
2	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	35
3	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	35
4	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	35
5	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	27





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

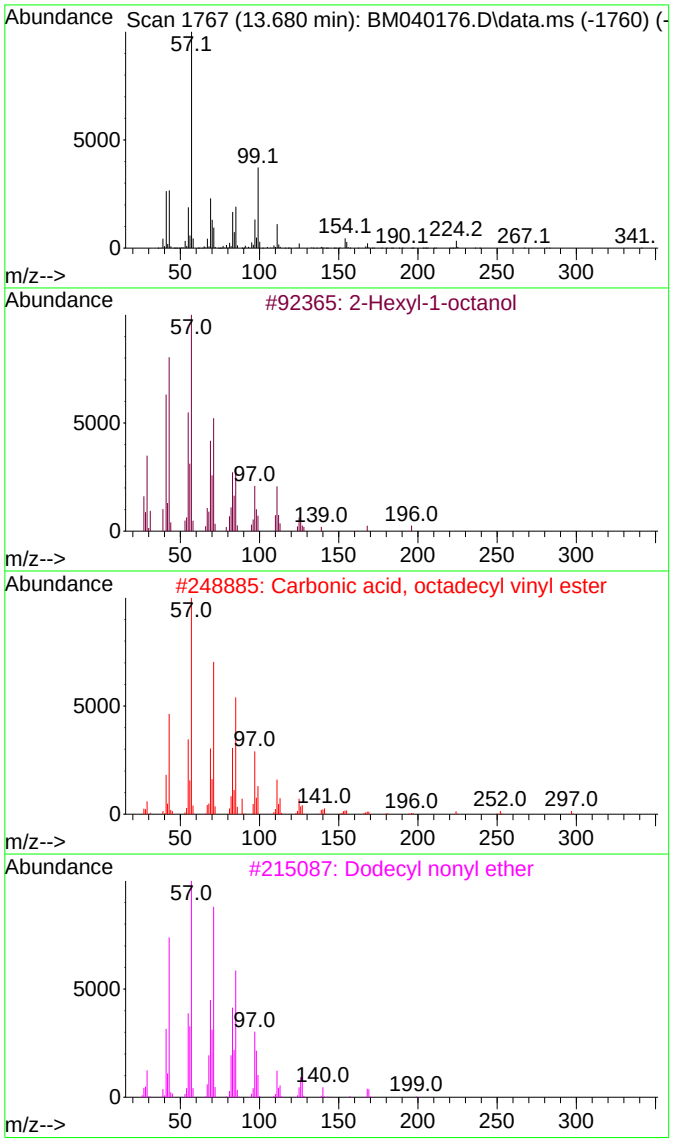
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

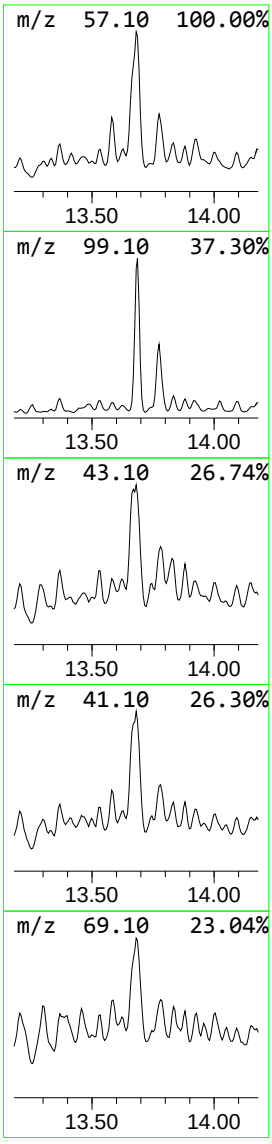
****

Peak Number 10 2-Hexyl-1-octanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.681	144.65 ng	25487600	Acenaphthene-d10	14.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexyl-1-octanol	214	C14H30O	019780-79-1	59
2	Carbonic acid, octadecyl vinyl e...	340	C21H40O3	1000382-54-4	53
3	Dodecyl nonyl ether	312	C21H44O	1000406-37-5	53
4	Carbonic acid, undecyl vinyl ester	242	C14H26O3	1000382-54-9	53
5	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	50





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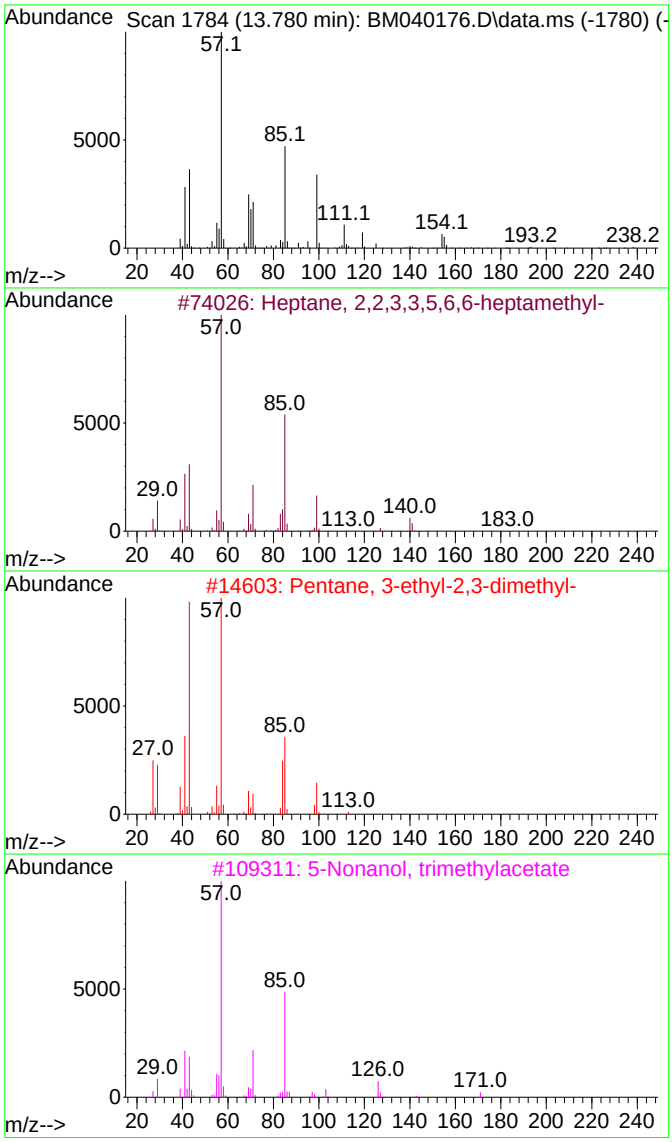
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

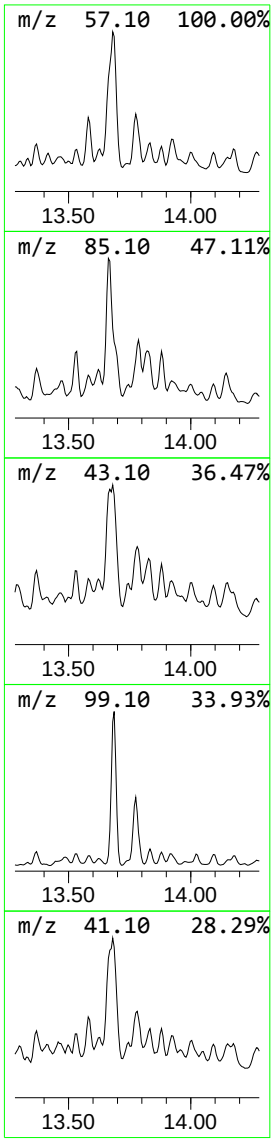
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Heptane, 2,2,3,3,5,6,6-hept... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.781	25.87 ng	4559120	Acenaphthene-d10	14.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2,2,3,3,5,6,6-heptamethyl-	198	C14H30	007225-67-4	50
2	Pentane, 3-ethyl-2,3-dimethyl-	128	C9H20	016747-33-4	43
3	5-Nonanol, trimethylacetate	228	C14H28O2	1000463-48-2	38
4	Oxalic acid, 6-ethyloct-3-yl hep...	328	C19H36O4	1000309-34-5	37
5	Oxalic acid, bis(6-ethyloct-3-yl...	370	C22H42O4	1000309-34-6	37





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

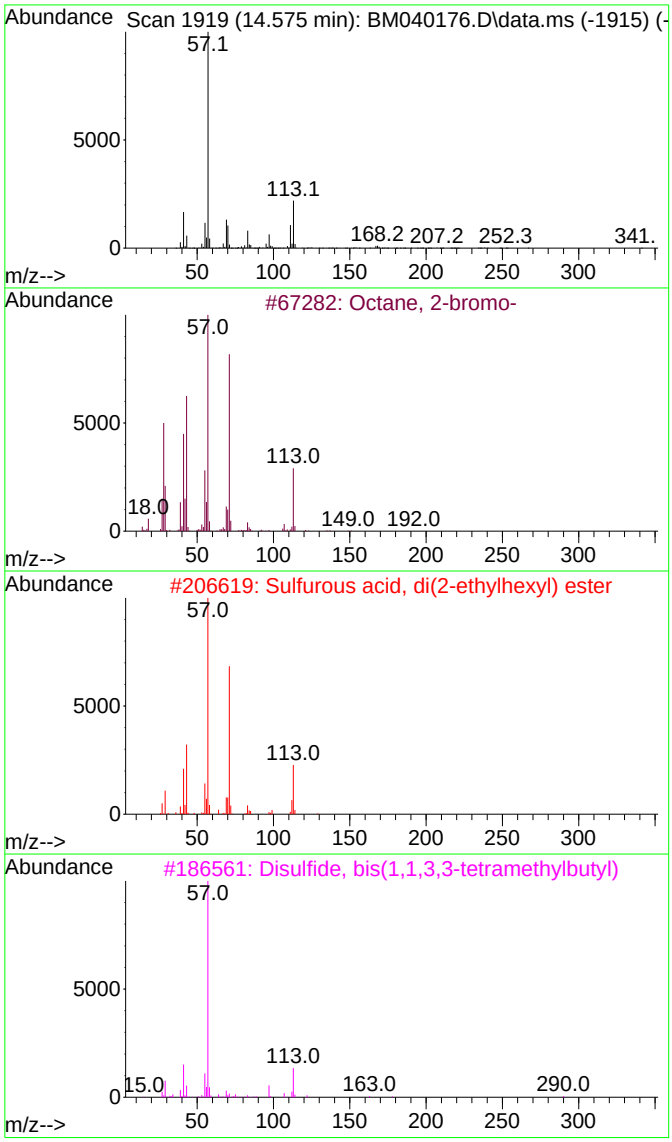
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

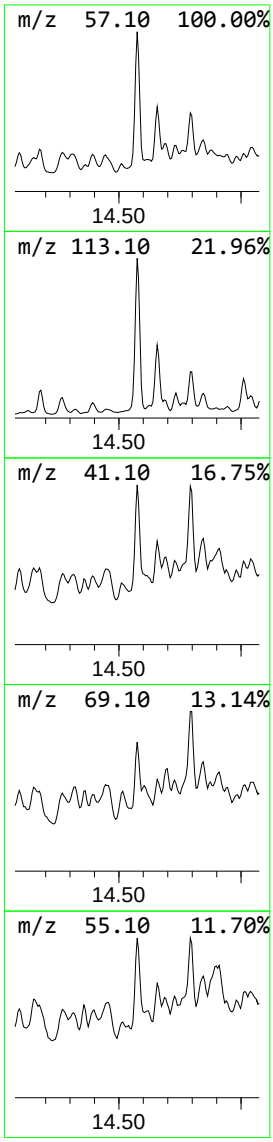
****

Peak Number 12 unknown14.575 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.575	46.71 ng	8229910	Acenaphthene-d10	14.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-bromo-	192	C8H17Br	000557-35-7	45
2	Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	40
3	Disulfide, bis(1,1,3,3-tetrameth...	290	C16H34S2	029956-99-8	38
4	Carbonic acid, but-2-yn-1-yl oct...	366	C23H42O3	1000383-21-3	37
5	Cyclopropanemethanol, .alpha.,2-...	156	C10H20O	056259-16-6	28





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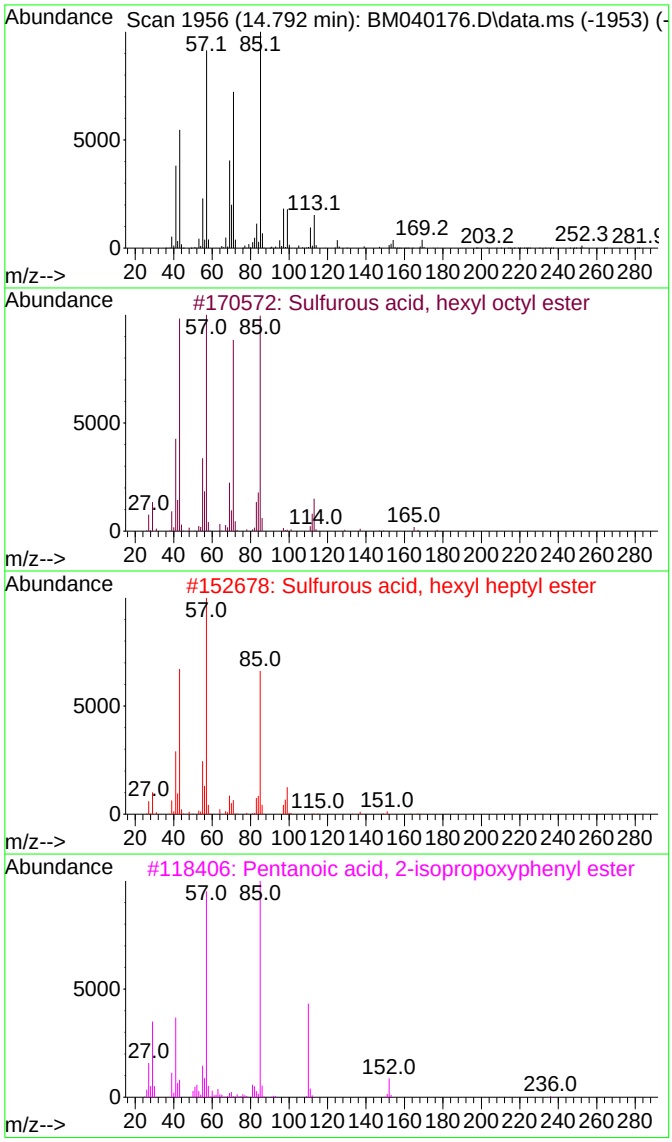
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

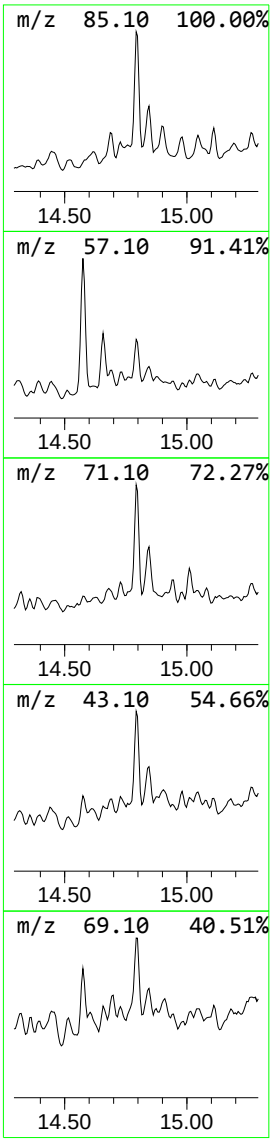
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Sulfurous acid, hexyl octyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.792	32.95 ng	5805840	Acenaphthene-d10	14.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	59
2	Sulfurous acid, hexyl heptyl ester	264	C13H28O3S	1000309-12-9	47
3	Pentanoic acid, 2-isopropoxyphen...	236	C14H20O3	1000293-64-6	43
4	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	43
5	Hentriacontane	437	C31H64	000630-04-6	43





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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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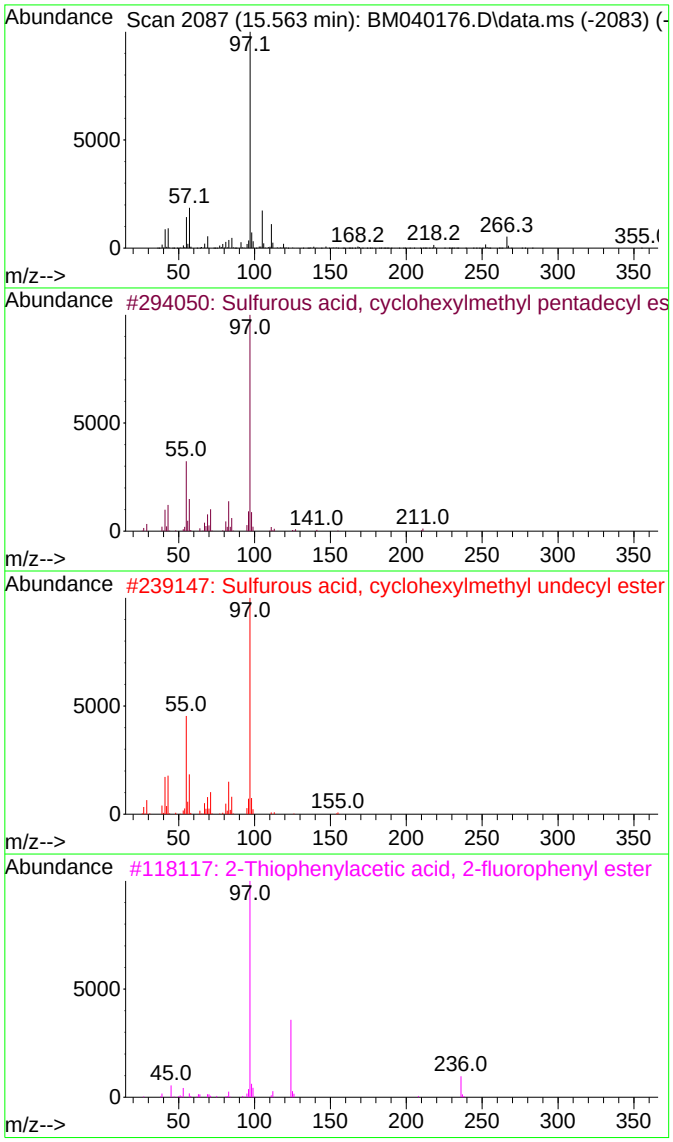
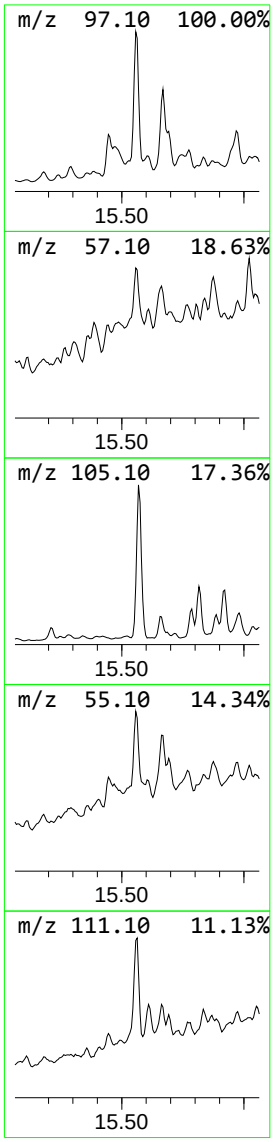
Peak Number 14 unknown15.563 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.563	60.86 ng	10724100	Acenaphthene-d10	14.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, cyclohexylmethyl...	388	C22H44O3S	1000309-22-3	42
2	Sulfurous acid, cyclohexylmethyl...	332	C18H36O3S	1000309-21-9	42
3	2-Thiophenylacetic acid, 2-fluor...	236	C12H9FO2S	1000325-71-6	40
4	7-Oxabicyclo[4.1.0]heptane, 1-me...	112	C7H12O	001713-33-3	39
5	2,4,4,6,6,8,8-Heptamethyl-2-nonene	224	C16H32	039761-73-4	38





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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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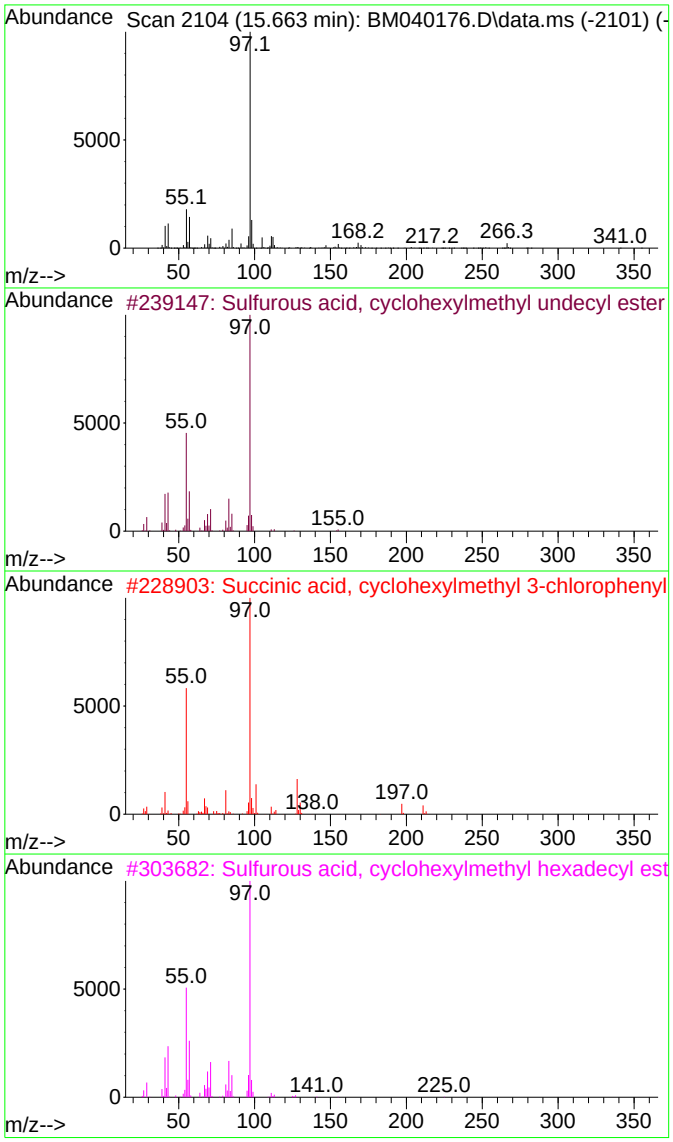
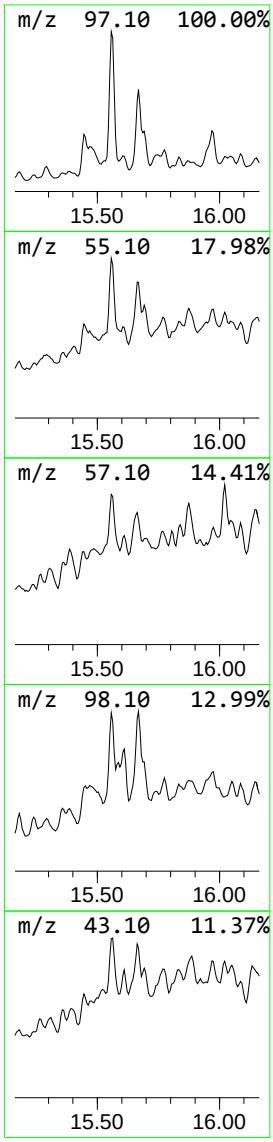
Peak Number 15 Sulfurous acid, cyclohexylm... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.663	27.86 ng	4908440	Acenaphthene-d10	14.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, cyclohexylmethyl...	332	C18H36O3S	1000309-21-9	64
2	Succinic acid, cyclohexylmethyl ...	324	C17H21ClO4	1010389-85-4	59
3	Sulfurous acid, cyclohexylmethyl...	402	C23H46O3S	1000309-22-4	56
4	Sulfurous acid, cyclohexylmethyl...	304	C16H32O3S	1000309-21-8	56
5	Sulfurous acid, cyclohexylmethyl...	388	C22H44O3S	1000309-22-3	56





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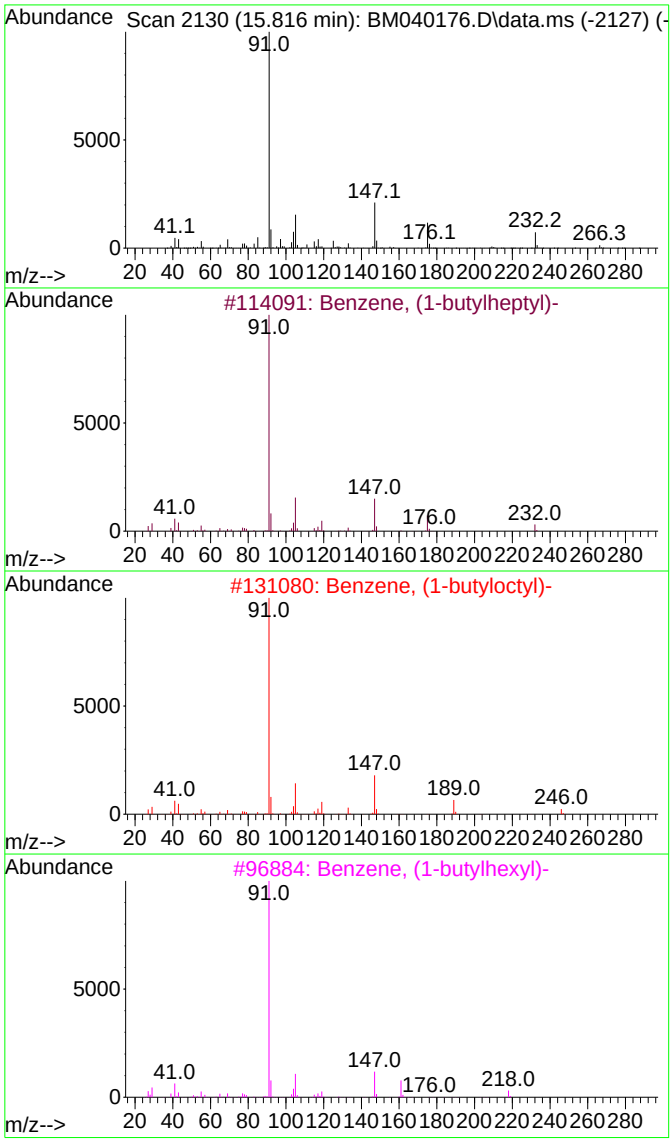
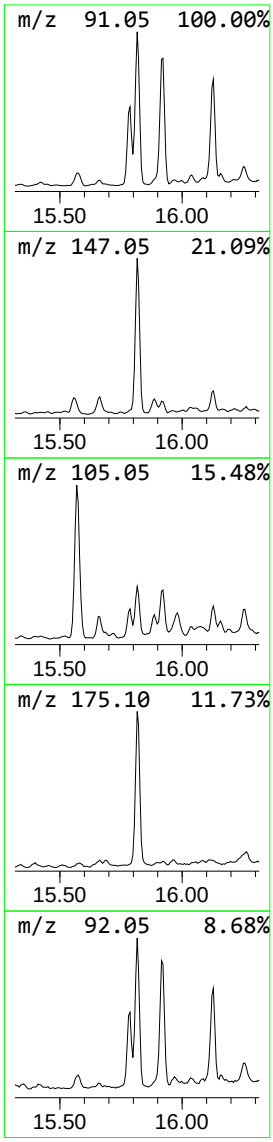
Peak Number 16 Benzene, (1-butylheptyl)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.816	27.82 ng	4901040	Acenaphthene-d10	14.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-butylheptyl)-	232	C17H28	004537-15-9	94
2	Benzene, (1-butyloctyl)-	246	C18H30	002719-63-3	59
3	Benzene, (1-butylhexyl)-	218	C16H26	004537-11-5	59
4	Benzene, (1,1-diethylpropyl)-	176	C13H20	004170-84-7	46
5	Solstitialin A	280	C15H20O5	022738-70-1	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060823\
Data File : BM040176.D
Acq On : 09 Jun 2023 02:57
Operator : MA/JU
Sample : 03046-07
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-2-6-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060823.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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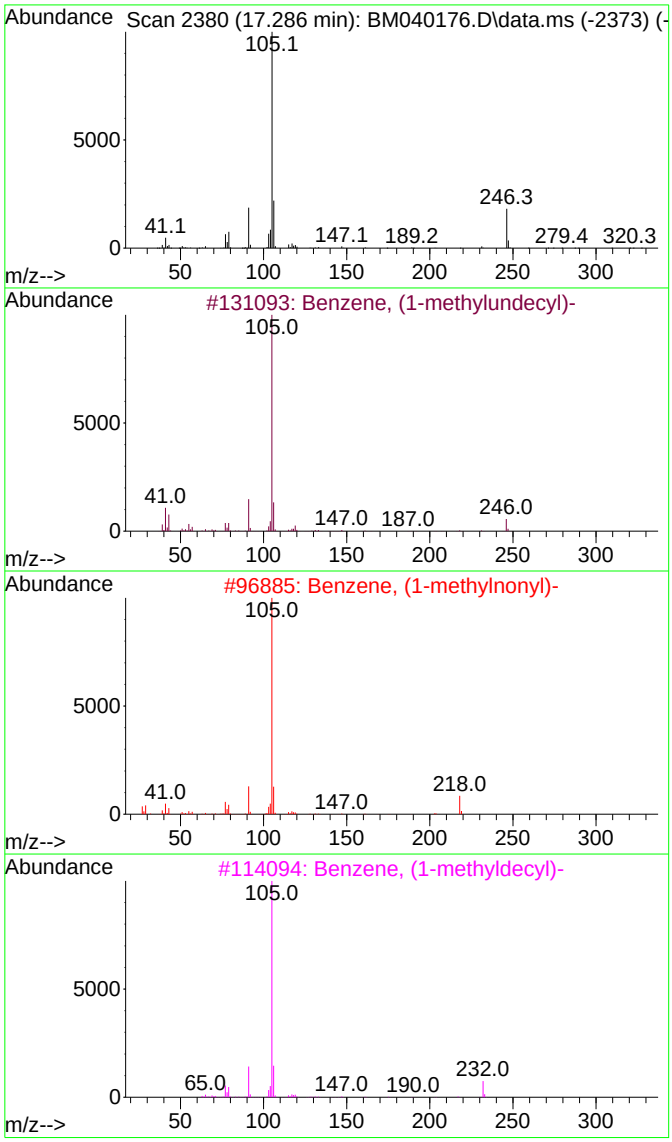
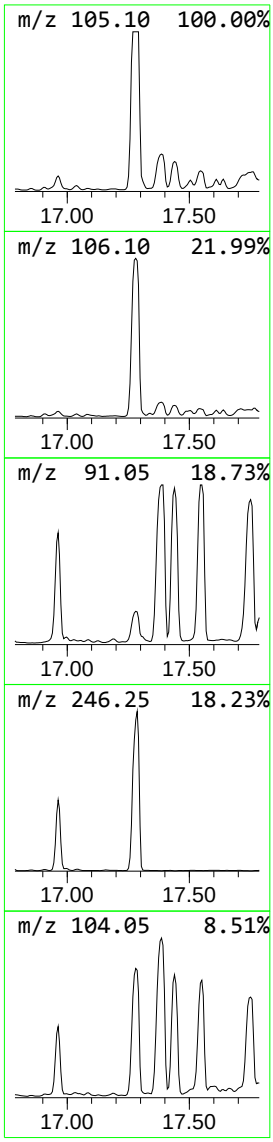
Peak Number 17 Benzene, (1-methylundecyl)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.286	29.63 ng	38444000	Phenanthrene-d10	17.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	59
2	Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	47
3	Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	47
4	(4-Methylphenyl) methanol, 1-met...	178	C12H18O	1000374-65-6	40
5	(3-Methylphenyl) methanol, 1-met...	178	C12H18O	1000374-58-5	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060823\
Data File : BM040176.D
Acq On : 09 Jun 2023 02:57
Operator : MA/JU
Sample : 03046-07
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-2-6-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060823.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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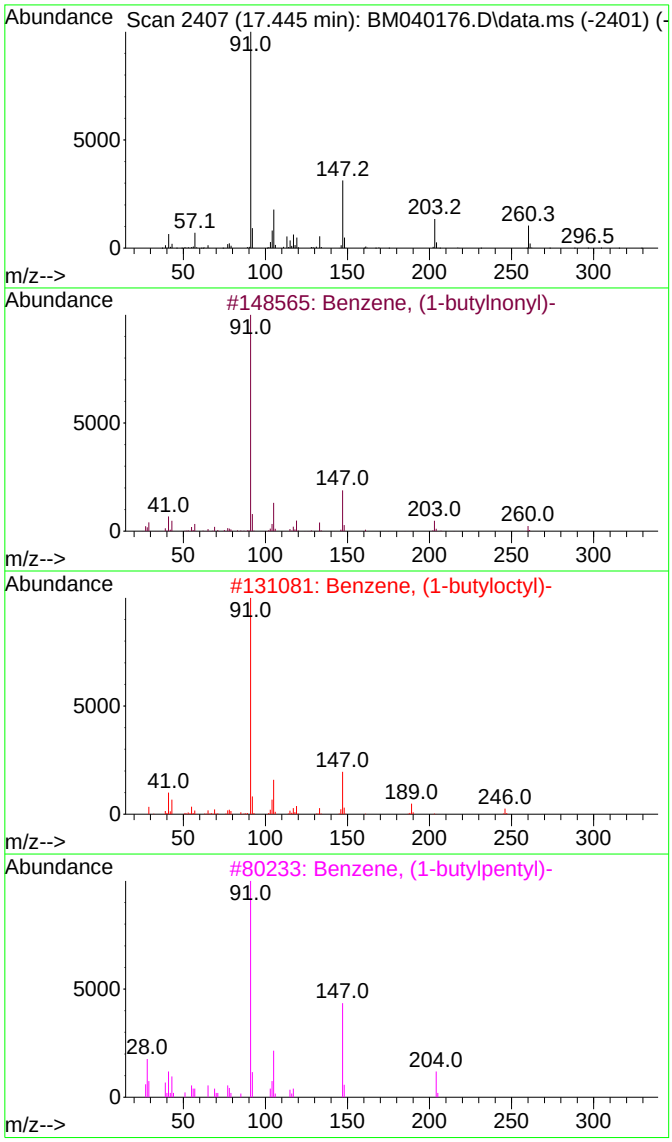
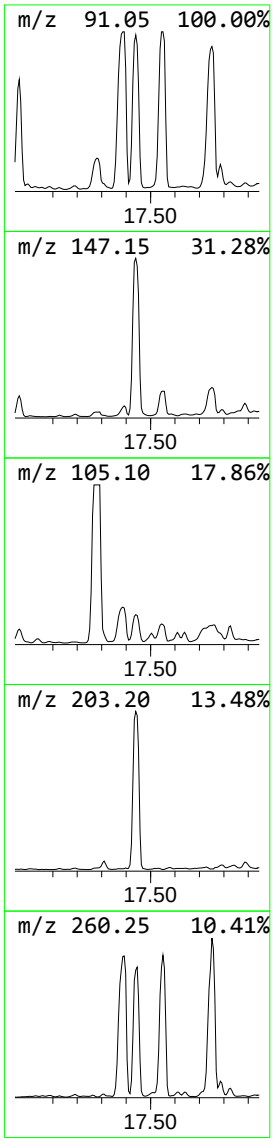
Peak Number 18 Benzene, (1-butylnonyl)- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.445	25.31 ng	32839900	Phenanthrene-d10	17.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-butylnonyl)-	260	C19H32	004534-50-3	90
2	Benzene, (1-butyloctyl)-	246	C18H30	002719-63-3	53
3	Benzene, (1-butylpentyl)-	204	C15H24	020216-88-0	50
4	Phenethyl isocyanate	147	C9H9NO	001943-82-4	47
5	Benzene, (1-butylheptyl)-	232	C17H28	004537-15-9	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060823\
Data File : BM040176.D
Acq On : 09 Jun 2023 02:57
Operator : MA/JU
Sample : 03046-07
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-2-6-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060823.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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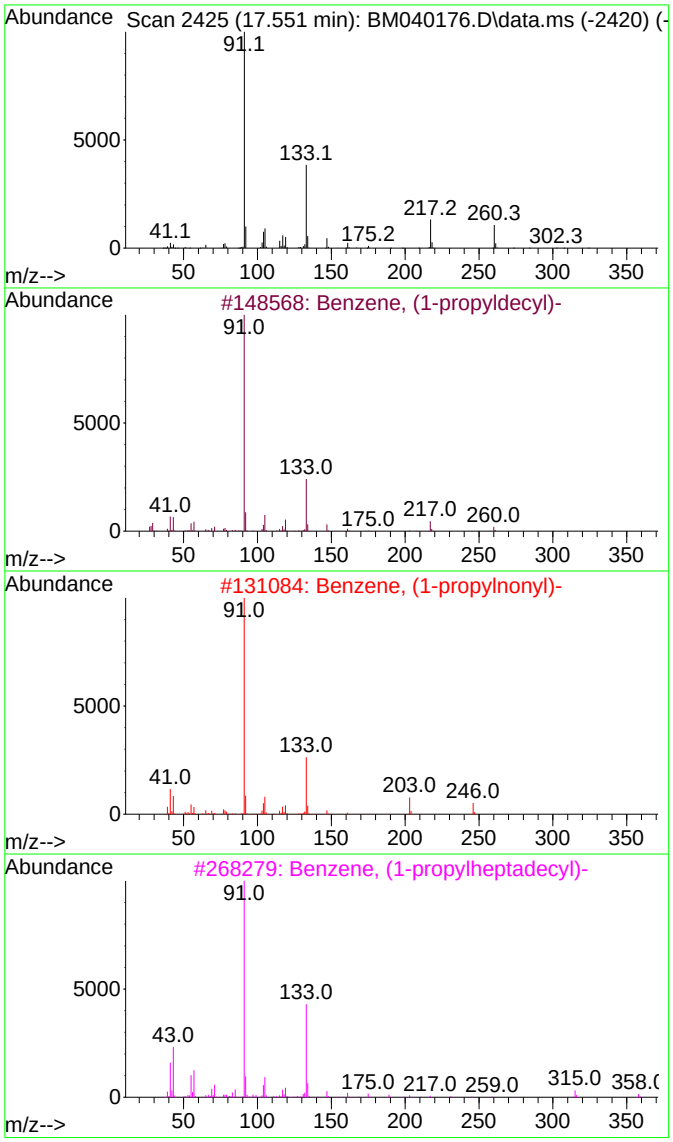
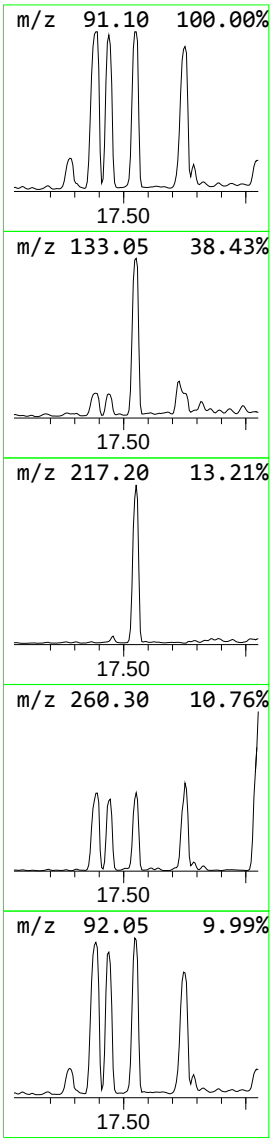
Peak Number 19 Benzene, (1-propyldecyl)- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.551	21.13 ng	27413500	Phenanthrene-d10	17.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-propyldecyl)-	260	C19H32	004534-51-4	91
2	Benzene, (1-propylnonyl)-	246	C18H30	002719-64-4	64
3	Benzene, (1-propylheptadecyl)-	358	C26H46	002400-03-5	50
4	Benzene, (1-propyloctyl)-	232	C17H28	004536-86-1	43
5	Benzene, (1-propylheptyl)-	218	C16H26	004537-12-6	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060823\
Data File : BM040176.D
Acq On : 09 Jun 2023 02:57
Operator : MA/JU
Sample : 03046-07
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-2-6-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060823.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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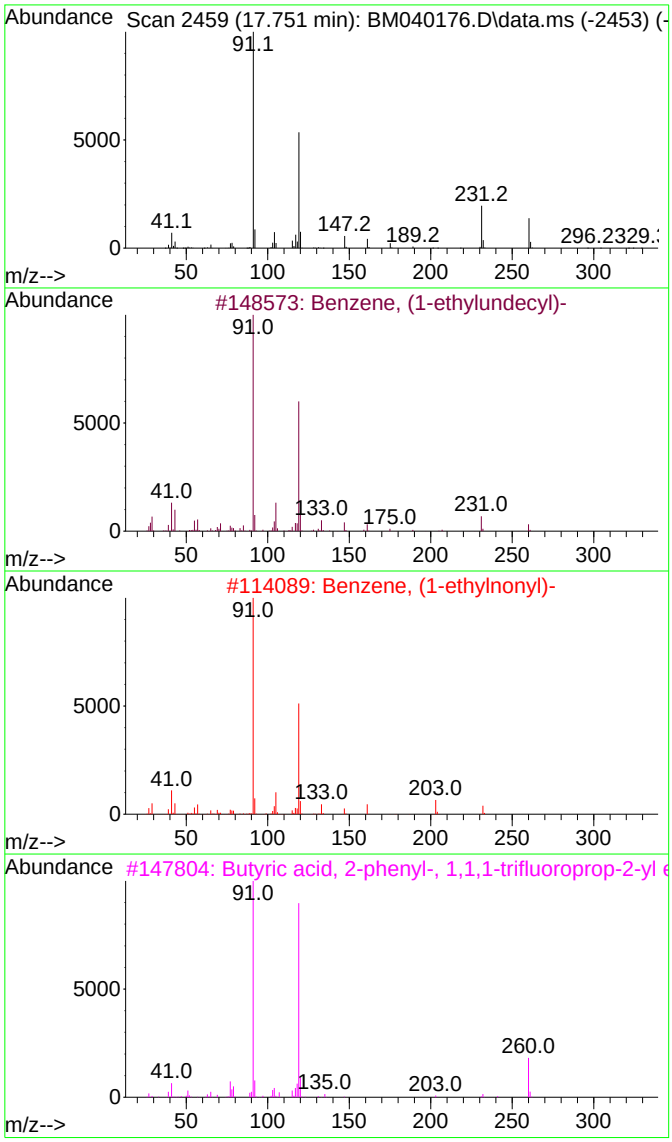
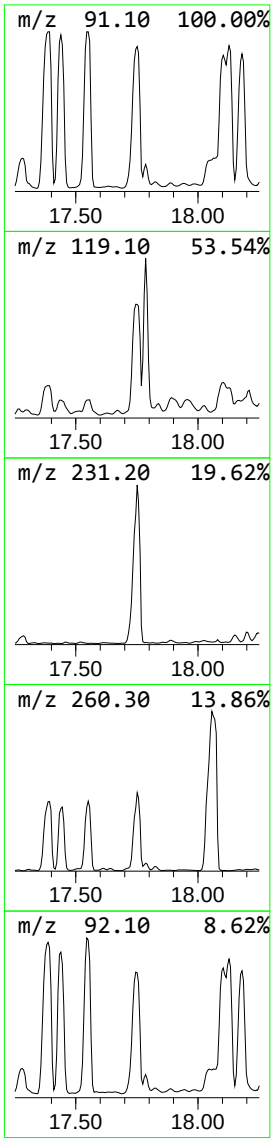
Peak Number 20 Benzene, (1-ethylundecyl)- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.751	23.42 ng	30397700	Phenanthrene-d10	17.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-ethylundecyl)-	260	C19H32	004534-52-5	94
2	Benzene, (1-ethylnonyl)-	232	C17H28	004536-87-2	58
3	Butyric acid, 2-phenyl-, 1,1,1-t...	260	C13H15F3O2	1000406-85-1	50
4	Benzene, (1-ethyldecyl)-	246	C18H30	002400-00-2	50
5	1-Chloro-2-methyl-2-phenylpropane	168	C10H13Cl	000515-40-2	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060823\
Data File : BM040176.D
Acq On : 09 Jun 2023 02:57
Operator : MA/JU
Sample : 03046-07
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-2-6-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060823.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
Acetoin	3.381	36.5	ng	4399690	1	7.987	2409140	20.0
Ethanol, 2-butoxy-	6.052	61.8	ng	7449600	1	7.987	2409140	20.0
Ethanol, 2-phen...	11.157	29.6	ng	5683160	2	10.804	3841160	20.0
Isoxazole, 3,5-...	12.034	34.4	ng	6601920	2	10.804	3841160	20.0
Sulfurous acid,...	12.945	32.7	ng	5760960	3	14.628	3524000	20.0
1H-Pyrazole, 5-...	13.051	36.1	ng	6366070	3	14.628	3524000	20.0
Carbonic acid, ...	13.151	36.1	ng	6360900	3	14.628	3524000	20.0
unknown13.369	13.369	23.9	ng	4206370	3	14.628	3524000	20.0
unknown13.581	13.581	26.1	ng	4598520	3	14.628	3524000	20.0
2-Hexyl-1-octanol	13.681	144.7	ng	25487600	3	14.628	3524000	20.0
Heptane, 2,2,3,...	13.781	25.9	ng	4559120	3	14.628	3524000	20.0
unknown14.575	14.575	46.7	ng	8229910	3	14.628	3524000	20.0
Sulfurous acid,...	14.792	33.0	ng	5805840	3	14.628	3524000	20.0
unknown15.563	15.563	60.9	ng	10724100	3	14.628	3524000	20.0
Sulfurous acid,...	15.663	27.9	ng	4908440	3	14.628	3524000	20.0
Benzene, (1-but...	15.816	27.8	ng	4901040	3	14.628	3524000	20.0
Benzene, (1-met...	17.286	29.6	ng	38444000	4	17.369	25953500	20.0
Benzene, (1-but...	17.445	25.3	ng	32839900	4	17.369	25953500	20.0
Benzene, (1-pro...	17.551	21.1	ng	27413500	4	17.369	25953500	20.0
Benzene, (1-eth...	17.751	23.4	ng	30397700	4	17.369	25953500	20.0