LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112021\
Data File : BP008059.D
Acq On : 20 Nov 2021 16:01
Operator : CG/JU
Sample : M4768-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-3

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-BP111921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008059.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.022	120	125	132	rBV	54029	77351	1.10%	0.171%
2	5.410	355	361	367	rBV	1262096	1832679	26.11%	4.063%
3	5.469	367	371	379	rVB	70068	140127	2.00%	0.311%
4	5.840	429	434	442	rBV	47946	74604	1.06%	0.165%
5	6.998	621	631	645	rBV	807858	1363092	19.42%	3.022%
6	7.822	764	771	779	rBV	488140	775027	11.04%	1.718%
7	8.192	829	834	843	rBV	178647	286001	4.07%	0.634%
8	8.469	875	881	886	rBV	67178	104810	1.49%	0.232%
9	8.934	950	960	962	rBV	107282	170748	2.43%	0.379%
10	8.981	962	968	986	rVB	1580939	2799372	39.88%	6.206%
11	9.169	994	1000	1009	rVB4	36806	82055	1.17%	0.182%
12	9.275	1009	1018	1032	rVB4	38895	111972	1.59%	0.248%
13	9.422	1032	1043	1045	rBV3	31025	76895	1.10%	0.170%
14	9.451	1045	1048	1054	rVB	62693	97606	1.39%	0.216%
15	9.816	1104	1110	1115	rBV	57827	99108	1.41%	0.220%
16	9.869	1115	1119	1123	rVV	73719	131571	1.87%	0.292%
17	10.022	1131	1145	1155	rBV2	163803	331870	4.73%	0.736%
18	10.410	1205	1211	1216	rBV2	42842	73585	1.05%	0.163%
19	10.616	1237	1246	1252	rBV	616883	1110370	15.82%	2.461%
20	10.675	1252	1256	1262	rVV4	118924	229595	3.27%	0.509%
21	10.739	1262	1267	1281	rVB2	102726	216774	3.09%	0.481%
22	11.086	1319	1326	1336	rVV	184997	310662	4.43%	0.689%
23	11.204	1338	1346	1352	rBV	200034	356343	5.08%	0.790%
24	11.533	1396	1402	1409	rVB3	67984	150943	2.15%	0.335%
25	11.728	1431	1435	1443	rVB3	67646	136653	1.95%	0.303%
26	11.810	1443	1449	1457	rBV6	42609	112987	1.61%	0.250%
27	11.951	1463	1473	1479	rBV4	59530	146602	2.09%	0.325%
28	12.175	1505	1511	1517	rVB3	110643	193901	2.76%	0.430%
29	12.257	1517	1525	1533	rBV5	42319	117793	1.68%	0.261%
30	12.498	1559	1566	1570	rBV	178764	301617	4.30%	0.669%
31	12.545	1570	1574	1578	rVV3	108623	183989	2.62%	0.408%
32	12.616	1583	1586	1591	rVB	65555	93011	1.32%	0.206%
33	12.804	1613	1618	1622	rBV5	39630	70284	1.00%	0.156%
34	12.951	1636	1643	1646	rBV6	33278	72518	1.03%	0.161%
35	13.086	1657	1666	1672	rBV	3607155	5301218	75.51%	11.752%
36	13.263	1691	1696	1699	rBV4	43998	85280	1.21%	0.189%

LSC Area Percent Report

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Data File : BP008059.D
Acq On : 20 Nov 2021 16:01
Operator : CG/JU
Sample : M4768-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-3

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-BP111921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.298	1699	1702	1711	rVB6	71850	131643	1.88%	0.292%
38	13.469	1727	1731	1735	rVB3	84664	120819	1.72%	0.268%
39	13.516	1735	1739	1743	rVB2	53117	79070	1.13%	0.175%
40	13.663	1759	1764	1773	rVB	141036	271689	3.87%	0.602%
41	13.792	1778	1786	1790	rBV5	105621	212575	3.03%	0.471%
42	13.957	1810	1814	1821	rBV3	50124	106957	1.52%	0.237%
43	14.022	1821	1825	1828	rBV5	57979	88218	1.26%	0.196%
44	14.180	1846	1852	1861	rVB5	60207	131484	1.87%	0.291%
45	14.463	1894	1900	1906	rBV	949563	1458248	20.77%	3.233%
46	14.527	1906	1911	1918	rVV2	166207	310236	4.42%	0.688%
47	14.616	1921	1926	1947	rVB	314670	624798	8.90%	1.385%
48	14.863	1964	1968	1975	rVB	72590	113115	1.61%	0.251%
49	15.080	1997	2005	2011	rBV4	145546	336902	4.80%	0.747%
50	15.286	2036	2040	2044	rBV2	79080	120802	1.72%	0.268%
51	15.351	2044	2051	2055	rVV	250292	421058	6.00%	0.933%
52	15.398	2055	2059	2068	rVB	183958	295380	4.21%	0.655%
53	15.510	2074	2078	2083	rVB	128202	181978	2.59%	0.403%
54	15.580	2084	2090	2096	rBV2	172386	309644	4.41%	0.686%
55	15.639	2096	2100	2103	rBV	102399	147740	2.10%	0.328%
56	15.727	2110	2115	2117	rBV5	58875	105494	1.50%	0.234%
57	15.827	2126	2132	2134	rBV4	154434	259500	3.70%	0.575%
58	15.957	2147	2154	2161	rBV	2763498	4224047	60.17%	9.364%
59	16.198	2190	2195	2203	rVB5	72033	159397	2.27%	0.353%
60	16.569	2255	2258	2262	rBV2	79531	111167	1.58%	0.246%
61	16.674	2273	2276	2283	rBV6	48089	105020	1.50%	0.233%
62	17.151	2354	2357	2363	rVB6	77018	114435	1.63%	0.254%
63	17.216	2363	2368	2374	rBV	1153876	1614327	22.99%	3.579%
64	17.416	2398	2402	2406	rBV3	95911	155797	2.22%	0.345%
65	17.510	2415	2418	2429	rVB2	42300	90582	1.29%	0.201%
66	17.621	2433	2437	2443	rVB	250256	342038	4.87%	0.758%
67	18.121	2517	2522	2529	rBV2	420979	732093	10.43%	1.623%
68	18.180	2530	2532	2541	rVB	85533	146151	2.08%	0.324%
69	18.421	2570	2573	2578	rVB	89192	118626	1.69%	0.263%
70	18.510	2584	2588	2596	rVB2	132048	262204	3.73%	0.581%
71	18.886	2649	2652	2657	rVB2	109277	150727	2.15%	0.334%
72	18.951	2658	2663	2670	rVV3	92252	217838	3.10%	0.483%
73	19.180	2698	2702	2705	rBV4	63664	90514	1.29%	0.201%
74	19.351	2727	2731	2740	rBV	267396	387372	5.52%	0.859%
75	19.474	2749	2752	2758	rVB4	68077	131302	1.87%	0.291%
76	19.786	2799	2805	2812	rBV	5636052	7020365	100.00%	15.563%

LSC Area Percent Report

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Acq On : 20 Nov 2021 16:01
Operator : CG/JU
Sample : M4768-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-3

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-BP111921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	21.027	3012	3016	3023	rBV3	210655	303019	4.32%	0.672%
78	21.092	3023	3027	3033	rBV	187000	253302	3.61%	0.562%
79	21.309	3059	3064	3068	rBV	1547958	1983569	28.25%	4.397%
80	22.415	3249	3252	3264	rVB	274642	414713	5.91%	0.919%
81	22.974	3343	3347	3351	rBV	140077	231858	3.30%	0.514%
82	23.698	3464	3470	3480	rVB2	1018216	2102877	29.95%	4.662%

Sum of corrected areas: 45109703

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112021\
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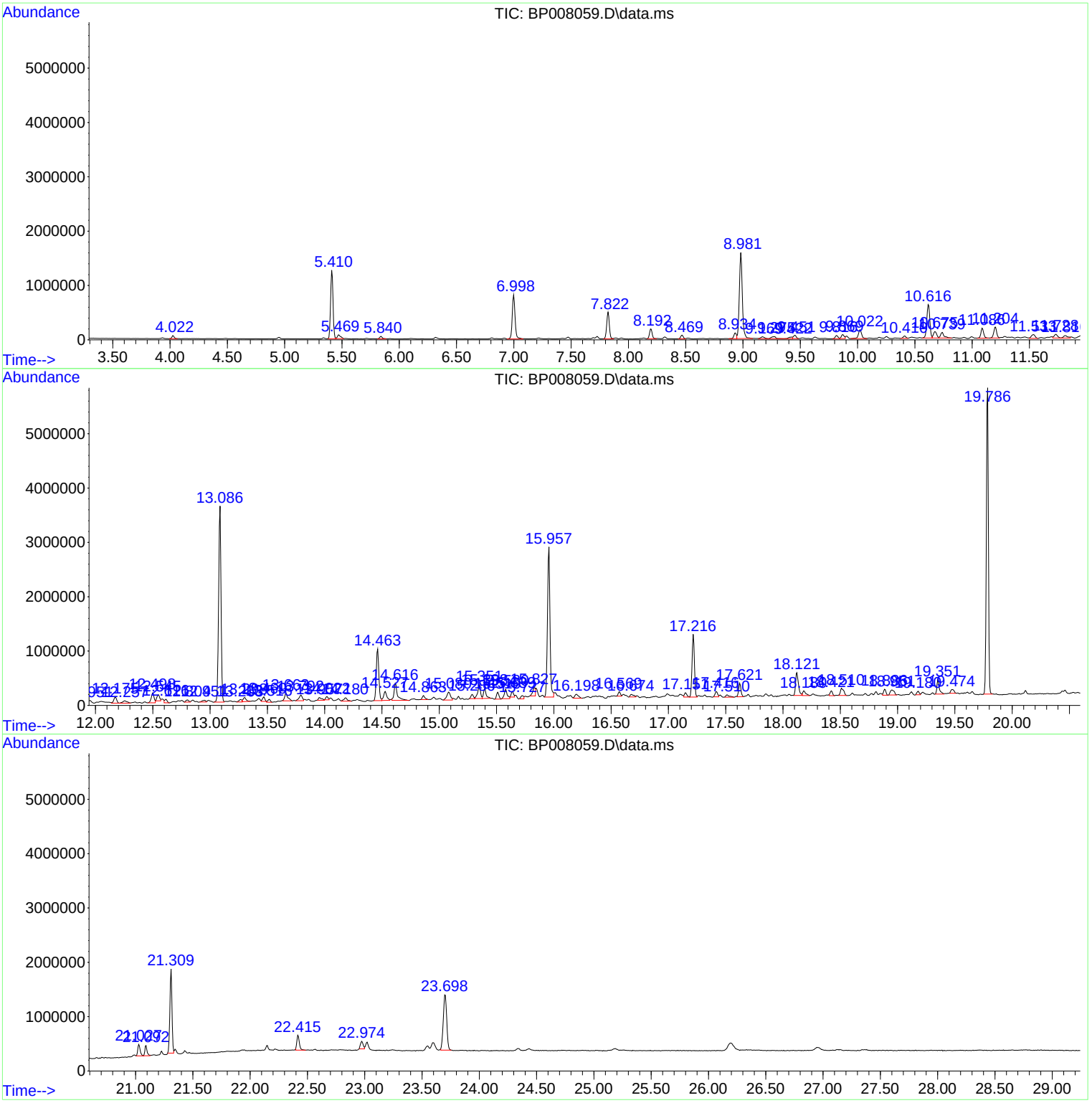
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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\BP112021\
Data File : BP008059.D
Acq On : 20 Nov 2021 16:01
Operator : CG/JU
Sample : M4768-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

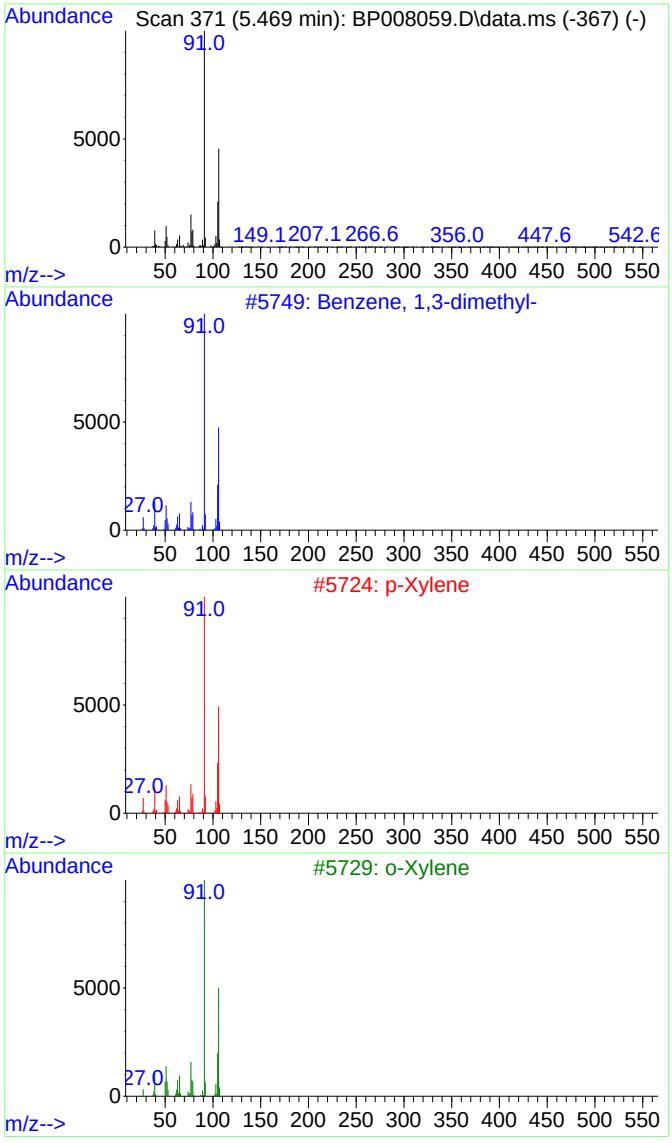
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

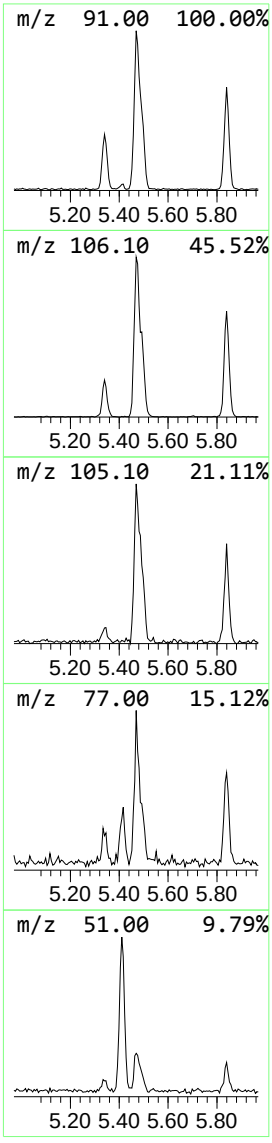
****

Peak Number 1 Benzene, 1,3-dimethyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.469	3.62 ng	140127	1,4-Dichlorobenzene-d4	7.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	90
2	p-Xylene	106	C8H10	000106-42-3	90
3	o-Xylene	106	C8H10	000095-47-6	87
4	Ethylbenzene	106	C8H10	000100-41-4	81
5	Cyclopentene, 1-ethenyl-3-methyl...	106	C8H10	061142-07-2	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112021\
Data File : BP008059.D
Acq On : 20 Nov 2021 16:01
Operator : CG/JU
Sample : M4768-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

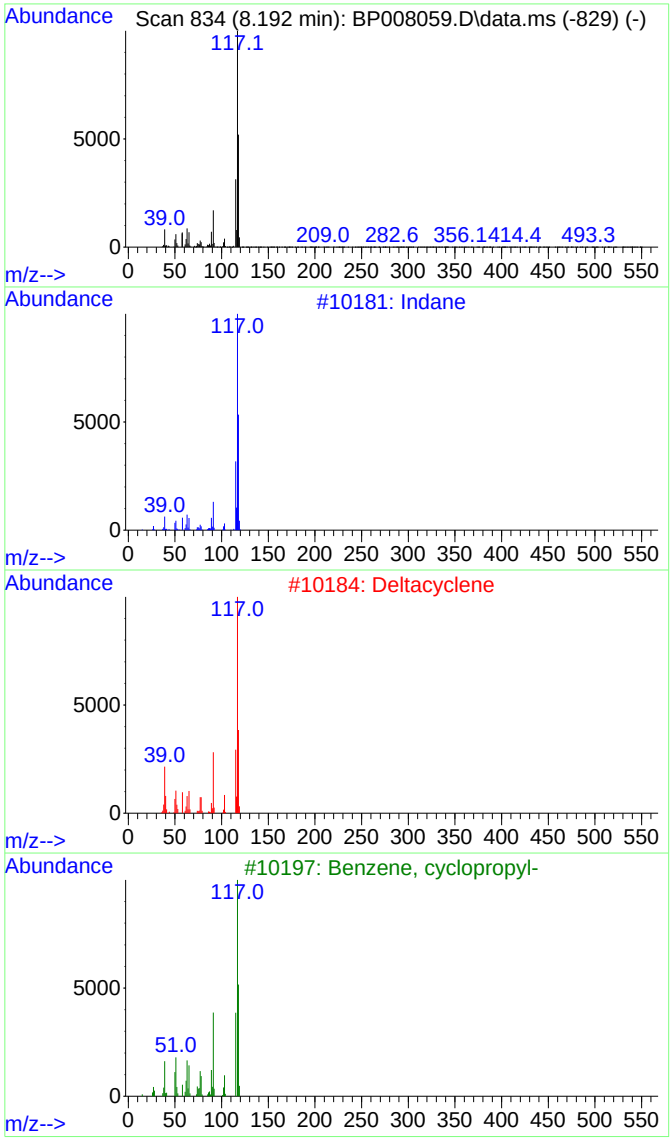
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

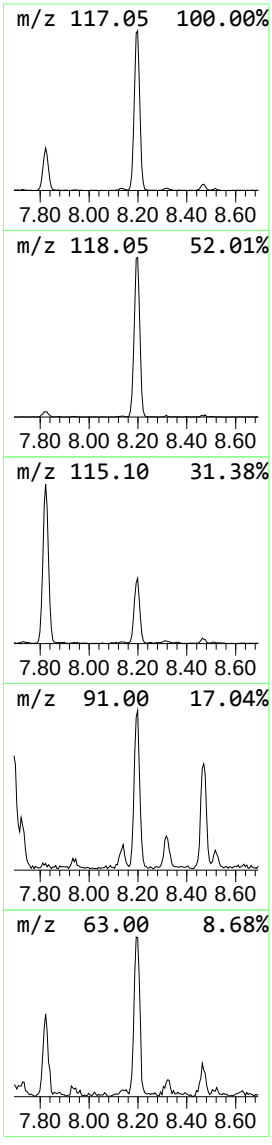
****

Peak Number 2 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.192	7.38 ng	286001	1,4-Dichlorobenzene-d4	7.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	91
2	Deltacyclene	118	C9H10	007785-10-6	64
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	60
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	59
5	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112021\
Data File : BP008059.D
Acq On : 20 Nov 2021 16:01
Operator : CG/JU
Sample : M4768-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

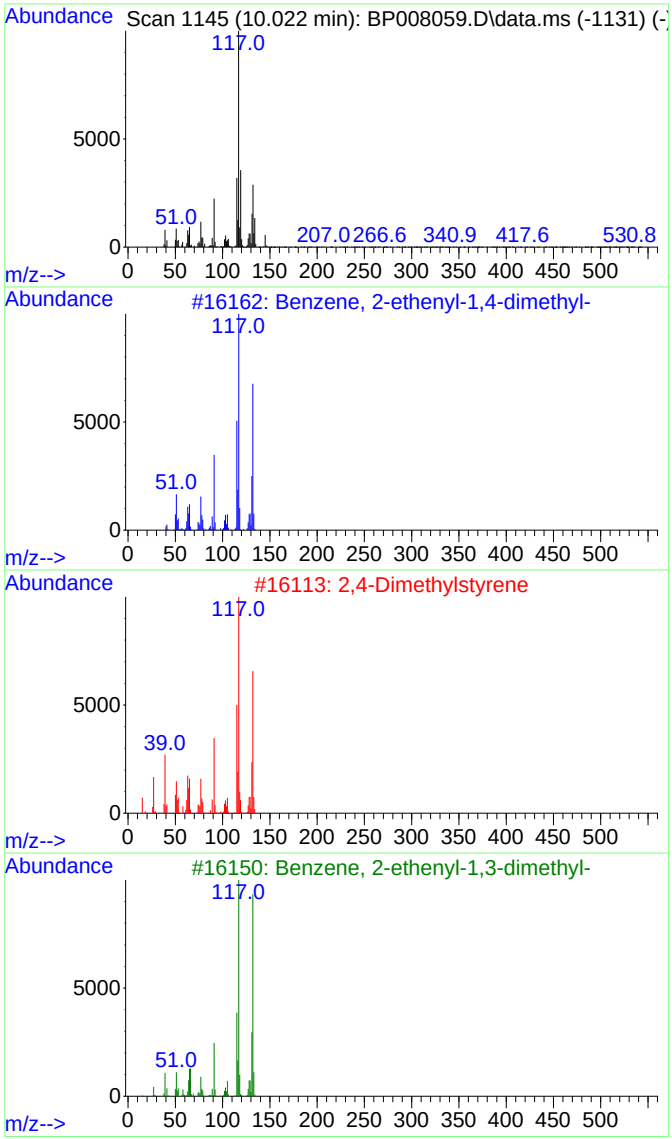
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

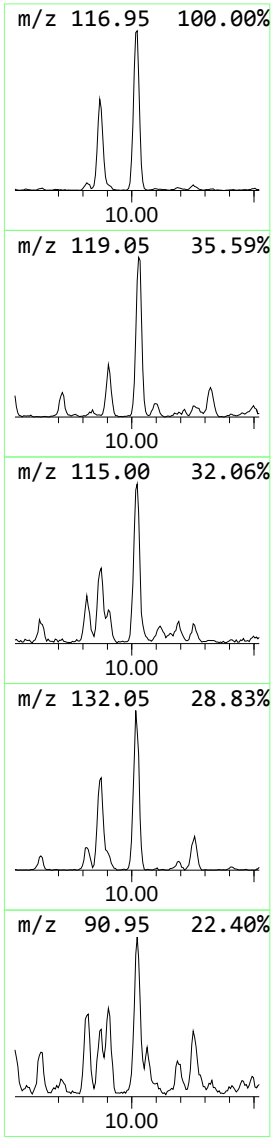
****

Peak Number 3 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.022	5.98 ng	331870	Naphthalene-d8	10.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
2	2,4-Dimethylstyrene	132	C10H12	002234-20-0	90
3	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	81
4	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	81
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112021\
Data File : BP008059.D
Acq On : 20 Nov 2021 16:01
Operator : CG/JU
Sample : M4768-01
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

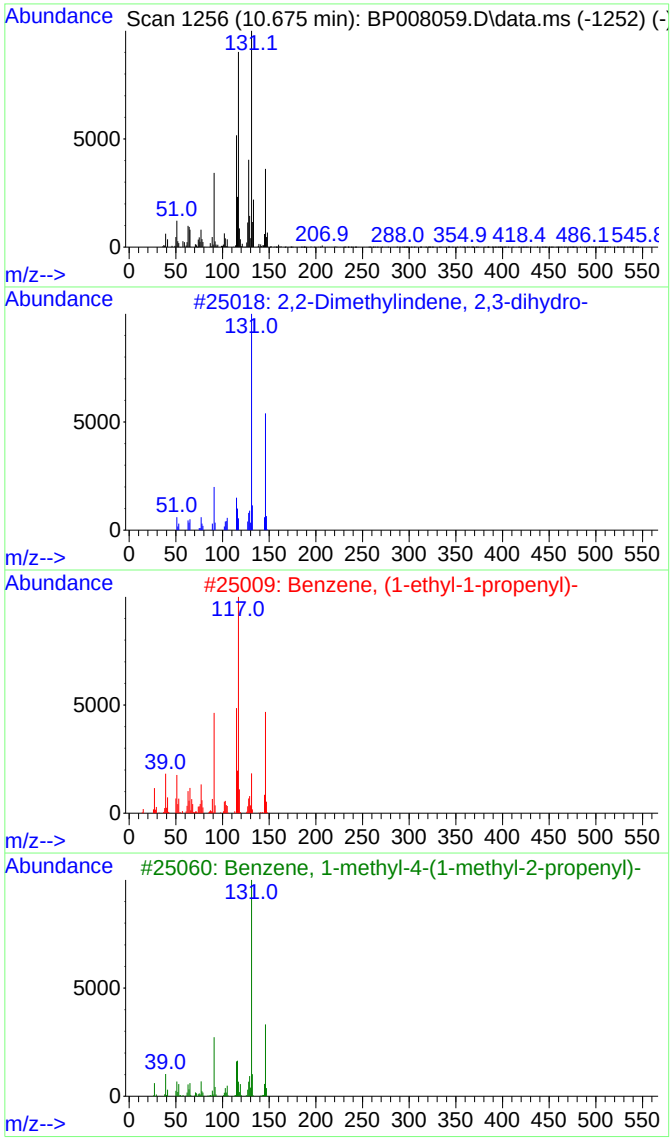
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

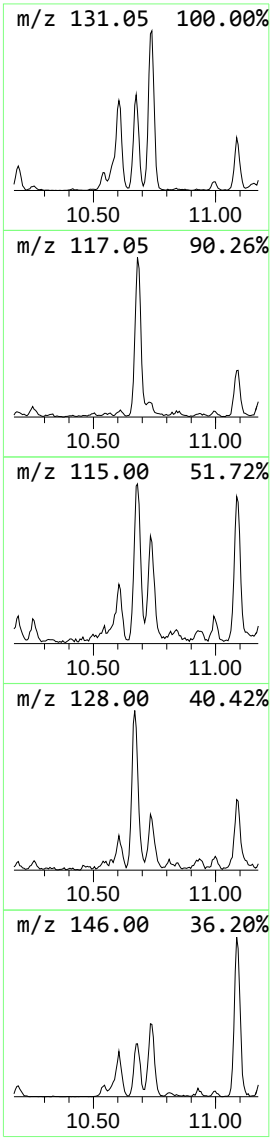
****

Peak Number 4 2,2-Dimethylindene, 2,3-dih... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.675	4.14 ng	229595	Naphthalene-d8	10.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	53
2	Benzene, (1-ethyl-1-propenyl)-	146	C11H14	004701-36-4	50
3	Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	43
4	trans-1-Phenyl-1-pentene	146	C11H14	016002-93-0	41
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	146	C11H14	027087-54-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112021\
Data File : BP008059.D
Acq On : 20 Nov 2021 16:01
Operator : CG/JU
Sample : M4768-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

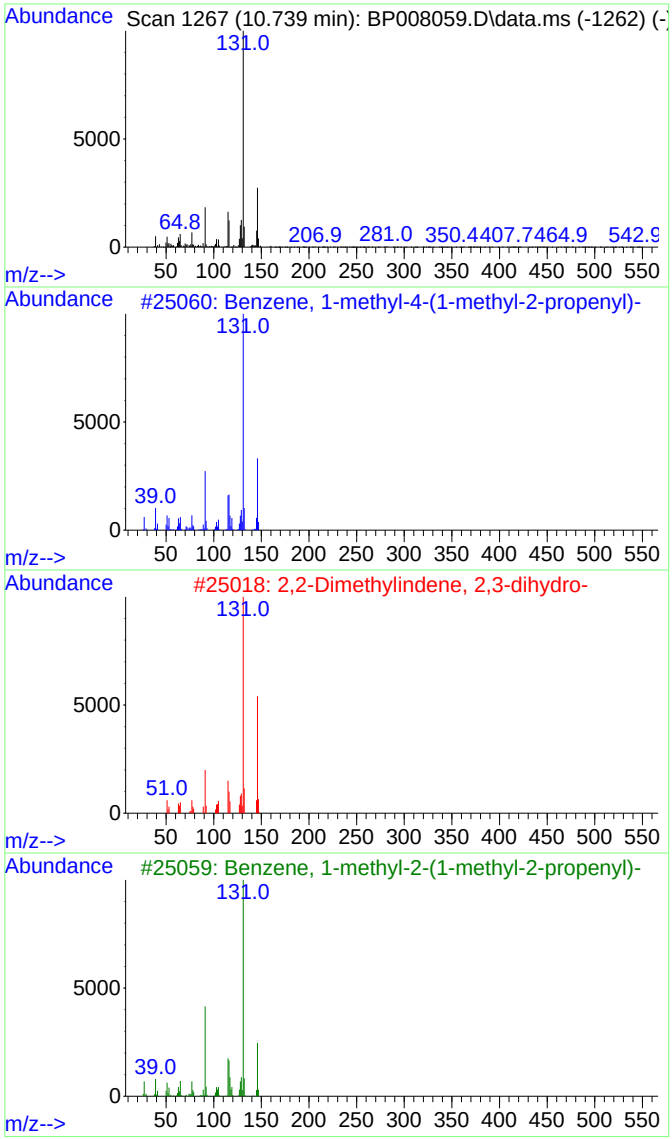
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

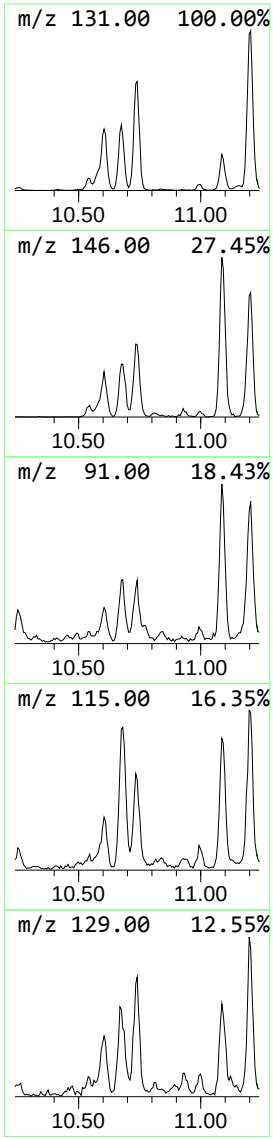
****

Peak Number 5 Benzene, 1-methyl-4-(1-meth... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.739	3.90 ng	216774	Naphthalene-d8	10.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	94
2	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	91
3	Benzene, 1-methyl-2-(1-methyl-2-...	146	C11H14	097664-19-2	91
4	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	91
5	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112021\
Data File : BP008059.D
Acq On : 20 Nov 2021 16:01
Operator : CG/JU
Sample : M4768-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-3

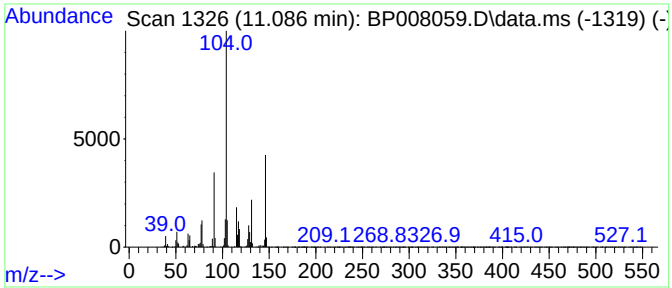
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

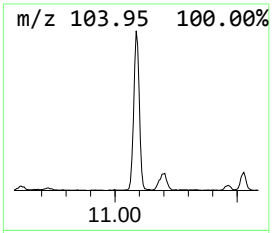
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

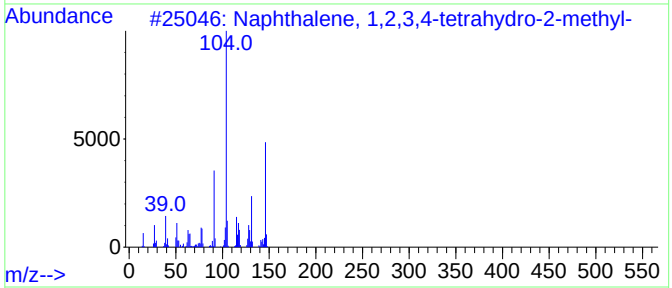
****
Peak Number 6 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 7

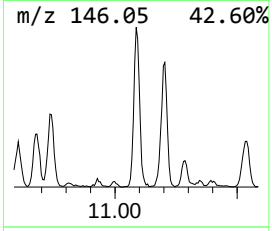
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.086	5.60 ng	310662	Naphthalene-d8	10.616

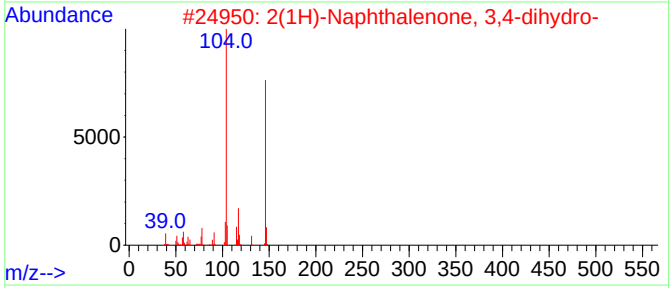
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	003877-19-8	94
2	2(1H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000530-93-8	64
3	Naphth[1,2-b]oxirene, 1a,2,3,7b-...	146	C10H10O	002461-34-9	62
4	2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	46
5	Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	007694-30-6	35

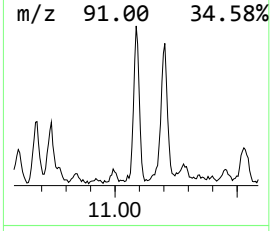


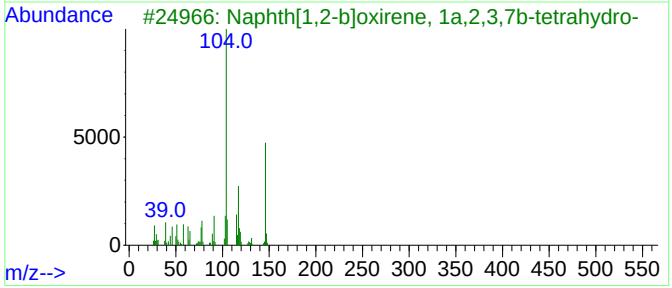


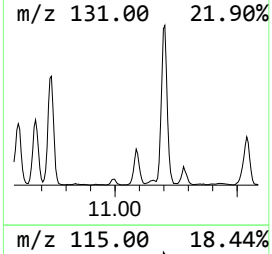


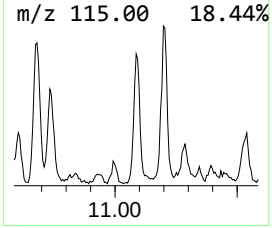












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Acq On : 20 Nov 2021 16:01
Operator : CG/JU
Sample : M4768-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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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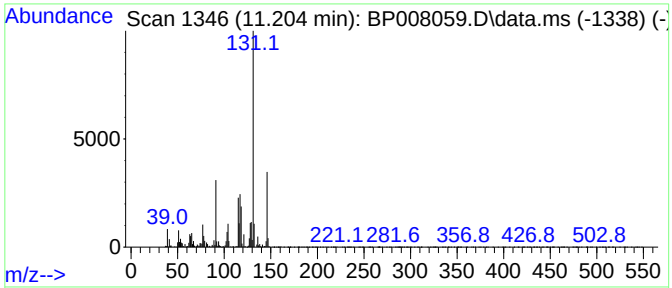
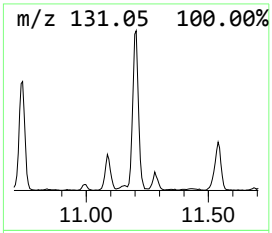
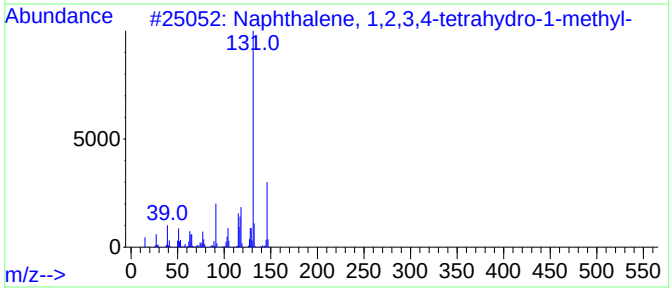
Peak Number 7 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 4

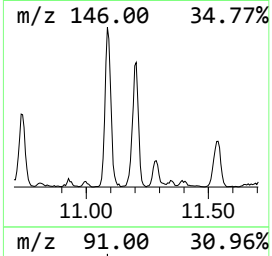
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.204	6.42 ng	356343	Naphthalene-d8	10.616

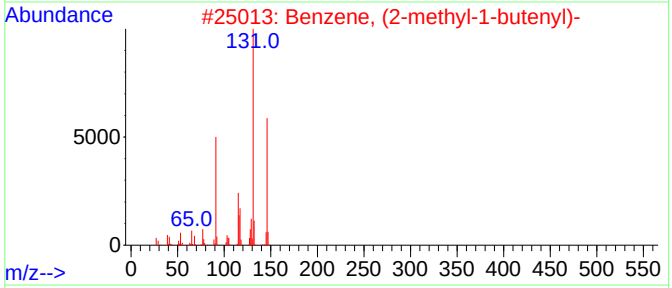
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	94
2	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	93
3	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	91
4	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	81
5	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	76

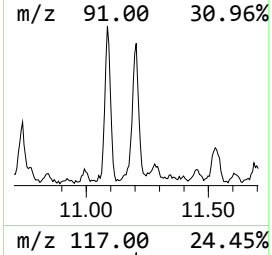


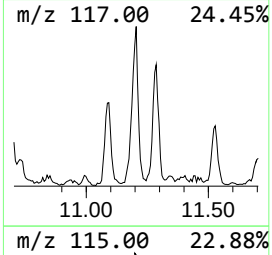


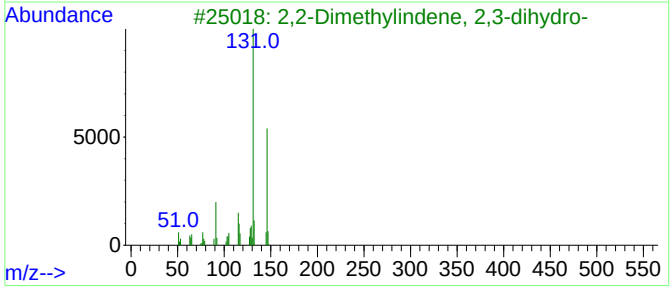


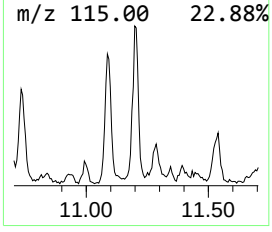












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Acq On : 20 Nov 2021 16:01
Operator : CG/JU
Sample : M4768-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-3

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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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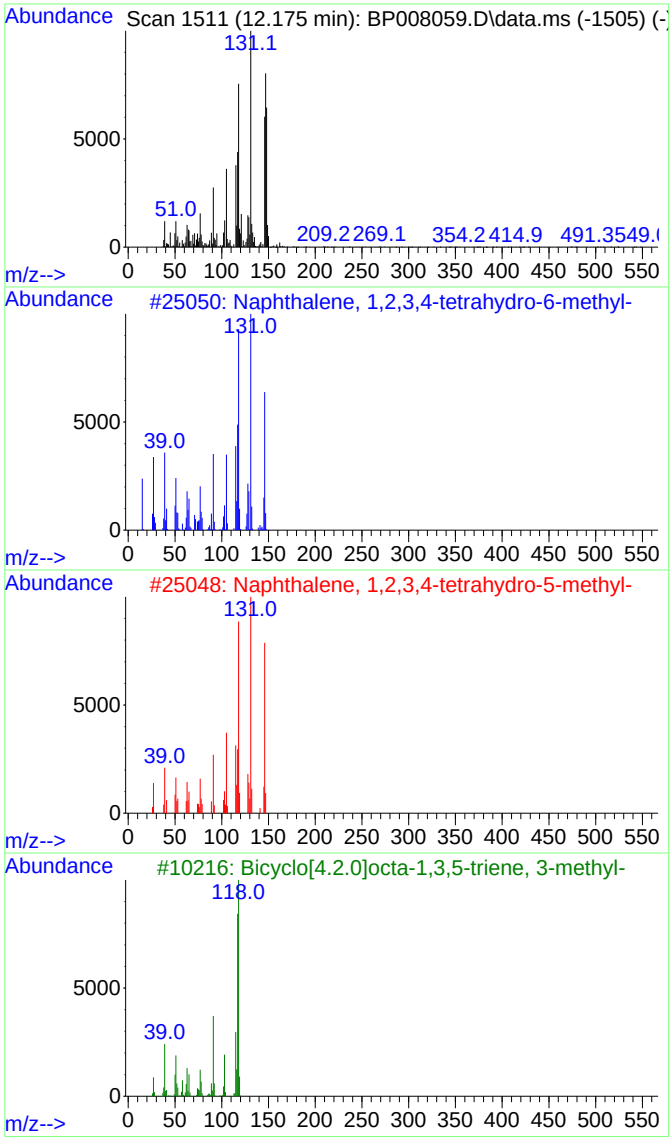
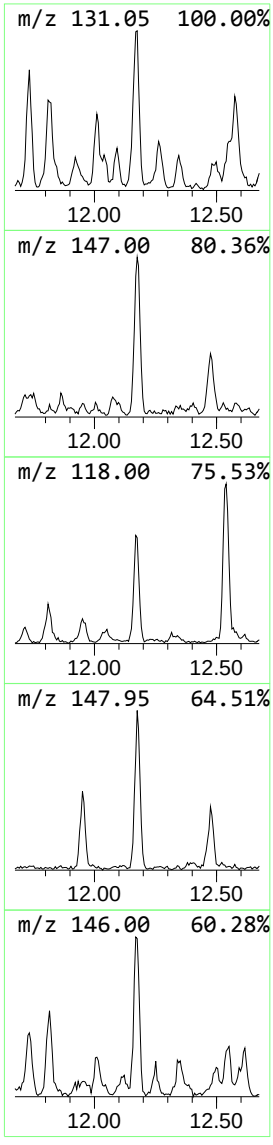
Peak Number 8 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.175	3.49 ng	193901	Naphthalene-d8	10.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	93
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	92
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	022250-74-4	64
4	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	42
5	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	42





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Sample : M4768-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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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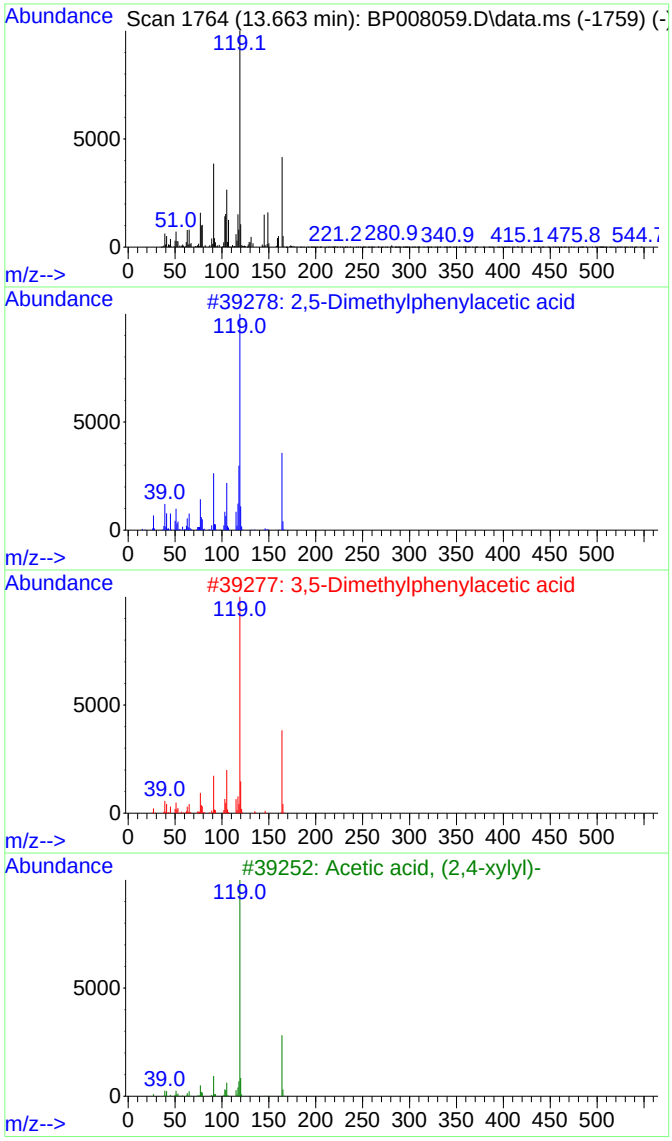
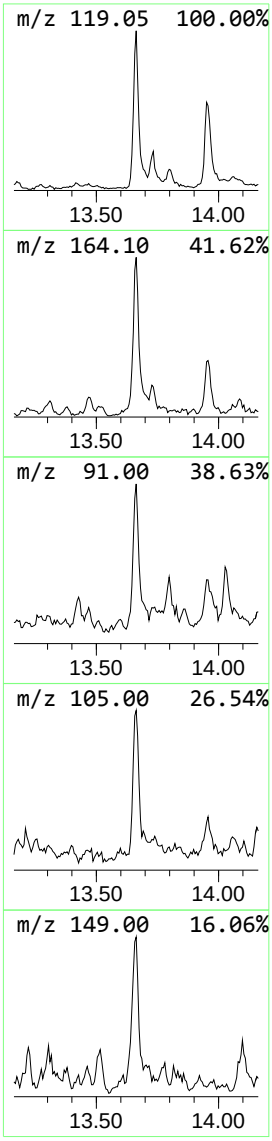
Peak Number 9 2,5-Dimethylphenylacetic acid Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.663	3.73 ng	271689	Acenaphthene-d10	14.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Dimethylphenylacetic acid	164	C10H12O2	1000342-65-5	83
2	3,5-Dimethylphenylacetic acid	164	C10H12O2	042288-46-0	64
3	Acetic acid, (2,4-xylyl)-	164	C10H12O2	006331-04-0	58
4	1,2-Phenylene bis(mesitylsulfonate)	474	C24H26O6S2	1000224-26-1	43
5	Butyric acid, 2-phenyl-, 4-chlor...	274	C16H15ClO2	1000406-87-4	43





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
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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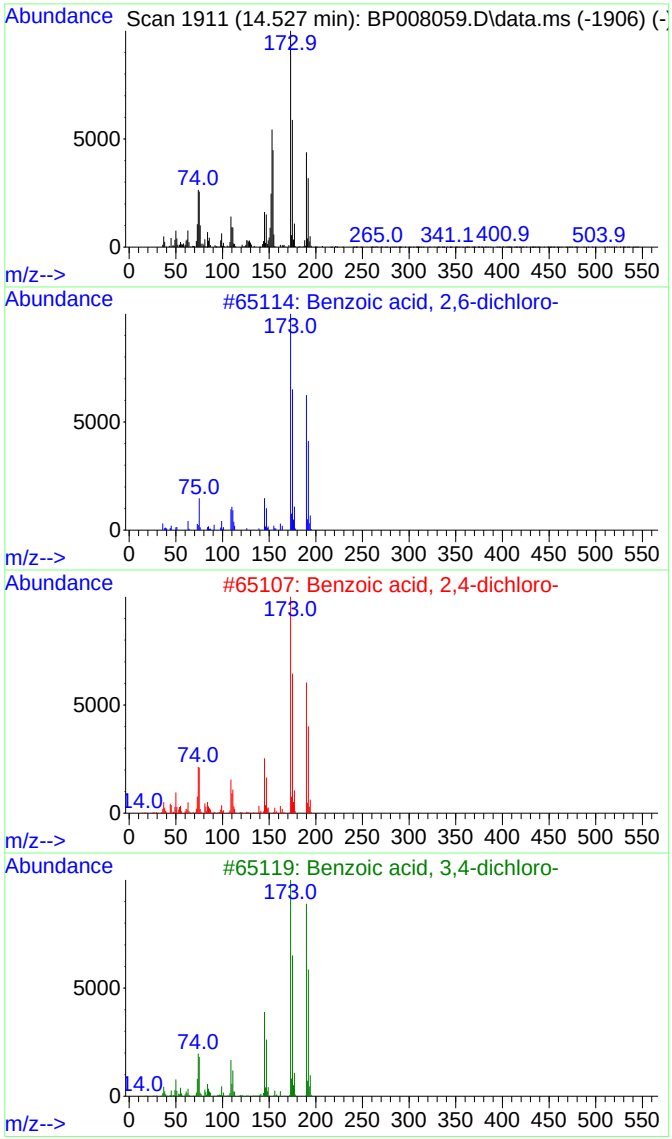
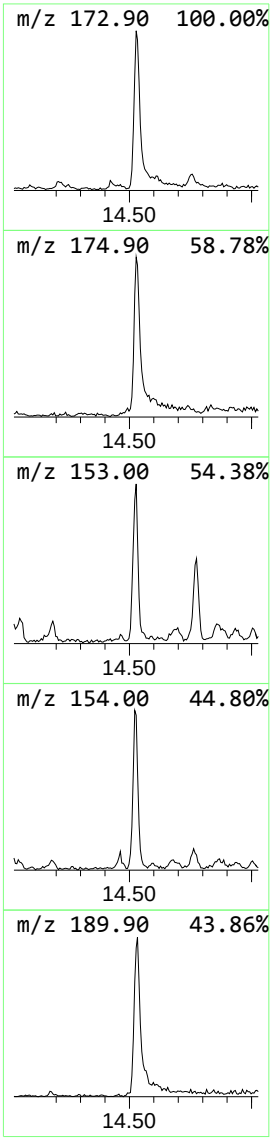
Peak Number 10 Benzoic acid, 2,6-dichloro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.527	4.25 ng	310236	Acenaphthene-d10	14.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,6-dichloro-	190	C7H4Cl2O2	000050-30-6	91
2	Benzoic acid, 2,4-dichloro-	190	C7H4Cl2O2	000050-84-0	89
3	Benzoic acid, 3,4-dichloro-	190	C7H4Cl2O2	000051-44-5	60
4	Benzoic acid, 2,5-dichloro-	190	C7H4Cl2O2	000050-79-3	53
5	Benzoic acid, 2,3-dichloro-	190	C7H4Cl2O2	000050-45-3	46





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
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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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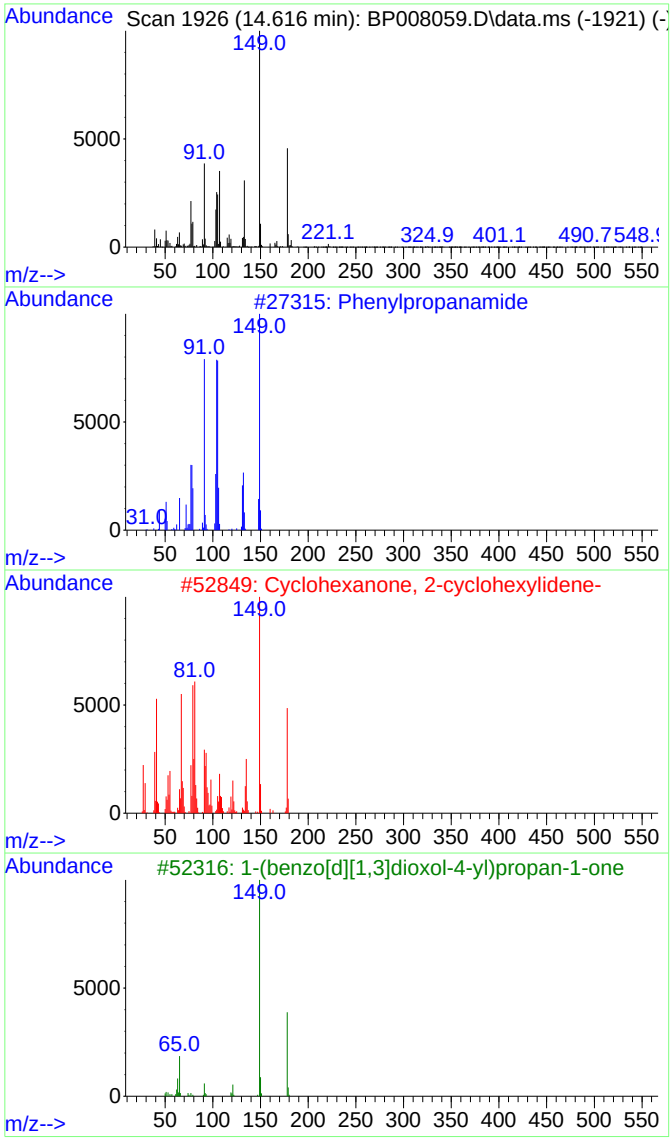
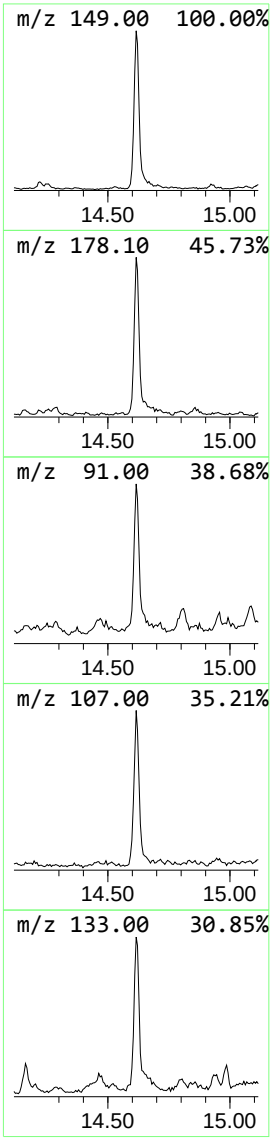
Peak Number 11 Phenylpropanamide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.616	8.57 ng	624798	Acenaphthene-d10	14.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenylpropanamide	149	C9H11NO	000102-93-2	52
2	Cyclohexanone, 2-cyclohexylidene-	178	C12H18O	001011-12-7	50
3	1-(benzo[d][1,3]dioxol-4-yl)prop...	178	C10H10O3	1000456-65-5	46
4	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	43
5	Phenyl(2-phenyl-1,3-dioxolan-2-y...	298	C18H18O4	006963-16-2	38





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ALS Vial : 7 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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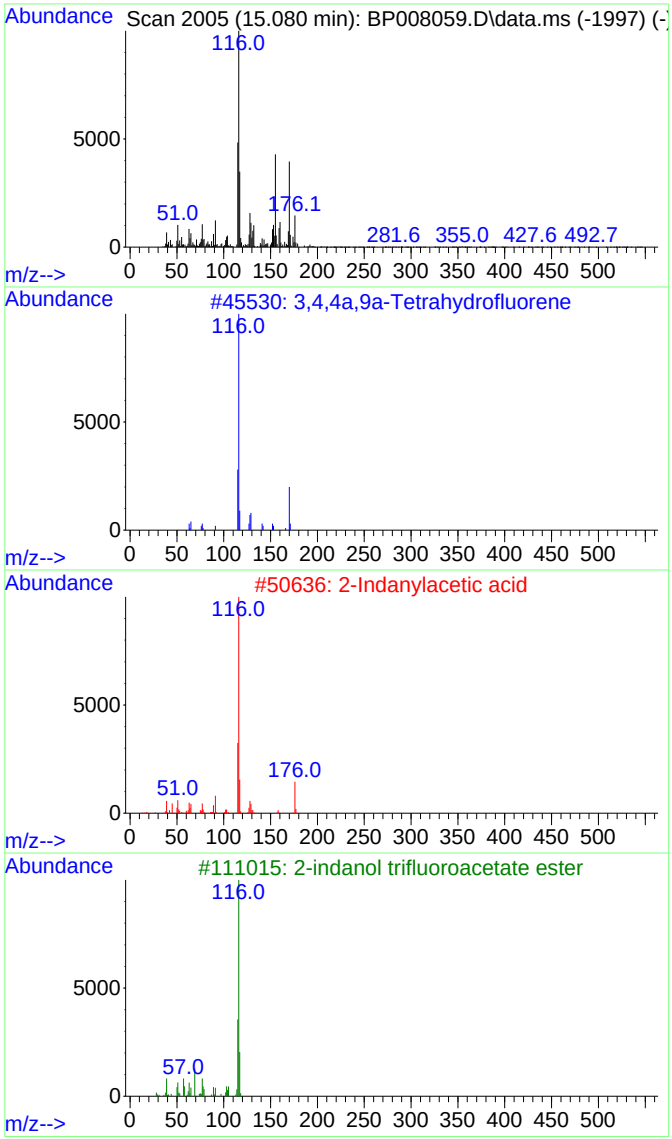
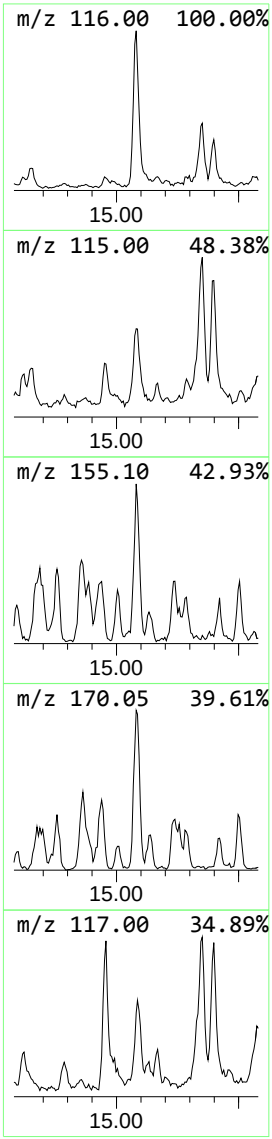
Peak Number 12 unknown15.080 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.080	4.62 ng	336902	Acenaphthene-d10	14.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4,4a,9a-Tetrahydrofluorene	170	C13H14	052652-40-1	49
2	2-Indanylacetic acid	176	C11H12O2	1000342-49-4	43
3	2-indanol trifluoroacetate ester	230	C11H9F3O2	1000376-43-8	38
4	trans-2-Phenylcyclopropylamine, ...	245	C11H10ClF2NO	1000447-48-6	38
5	2-Methoxy-2,3-dimethylbenzonorbo...	202	C14H18O	1010110-53-1	38





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ALS Vial : 7 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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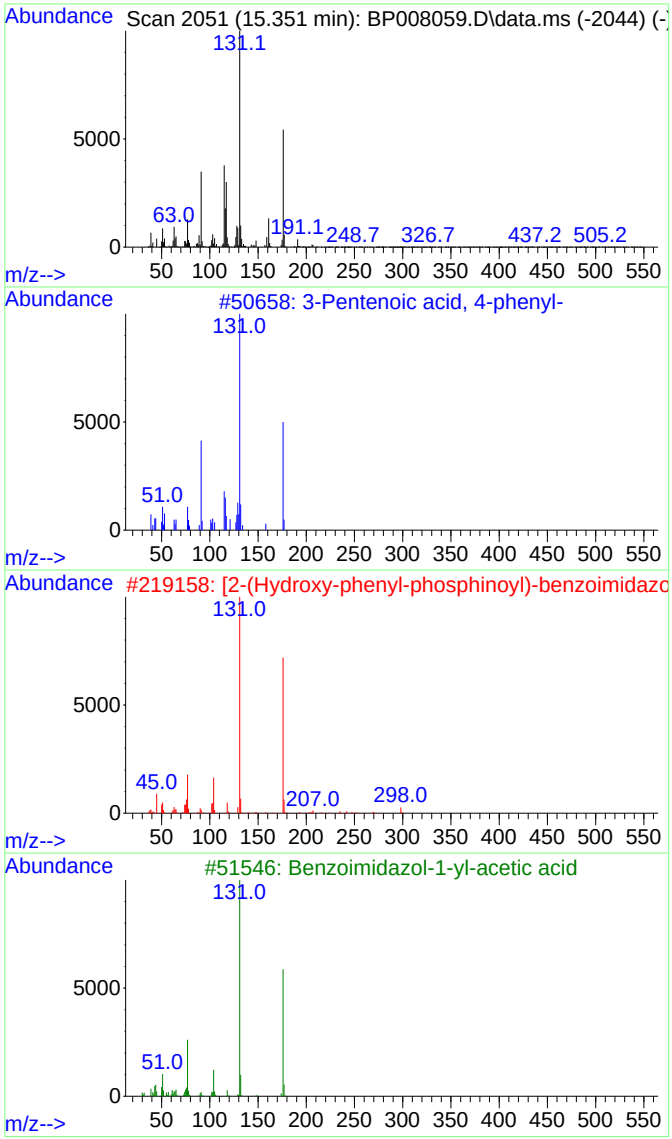
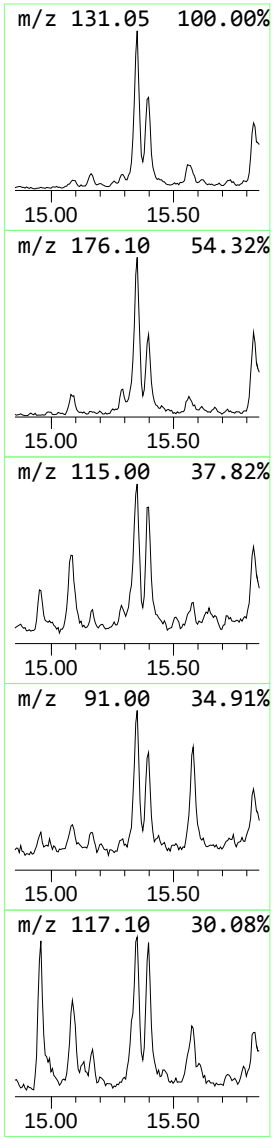
Peak Number 13 3-Pentenoic acid, 4-phenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.351	5.77 ng	421058	Acenaphthene-d10	14.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentenoic acid, 4-phenyl-	176	C11H12O2	053774-19-9	74
2	[2-(Hydroxy-phenyl-phosphinoyl)-...	316	C15H13N2O4P	300566-65-8	53
3	Benzoimidazol-1-yl-acetic acid	176	C9H8N2O2	1010317-79-2	53
4	5,6,7,8-Tetrahydro-2-naphthoic acid	176	C11H12O2	001131-63-1	50
5	Cyclopropane, 1-chloro-1-methyl-...	166	C10H11Cl	1000161-07-9	47





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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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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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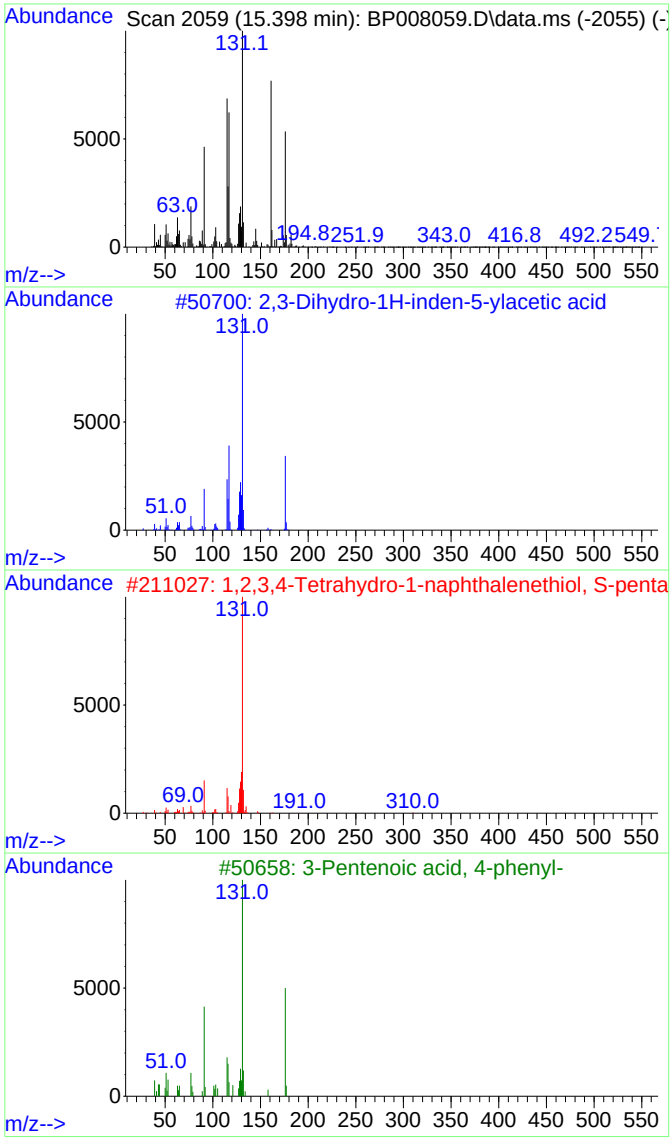
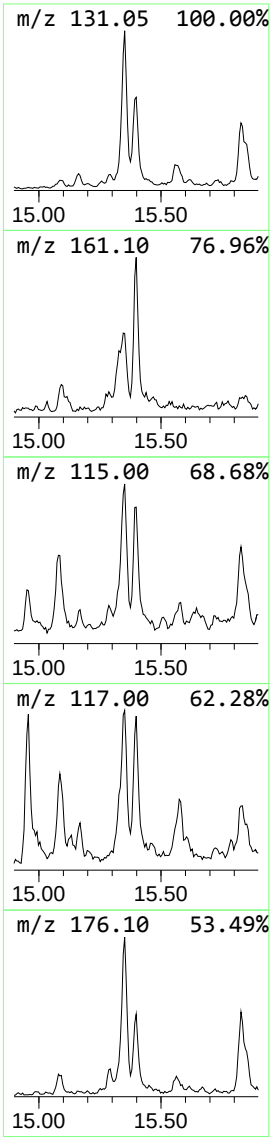
Peak Number 14 2,3-Dihydro-1H-inden-5-ylac... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.398	4.05 ng	295380	Acenaphthene-d10	14.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Dihydro-1H-inden-5-ylacetic ...	176	C11H12O2	005453-98-5	86
2	1,2,3,4-Tetrahydro-1-naphthalene...	310	C13H11F5OS	1000470-19-7	46
3	3-Pentenoic acid, 4-phenyl-	176	C11H12O2	053774-19-9	43
4	1(2H)-Naphthalenone, 3,4-dihydro...	161	C10H11NO	003349-64-2	35
5	Benzene, (3-chloro-1-methyl-1-pr...	166	C10H11Cl	1000327-43-7	35





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ClientSampleId :
MW-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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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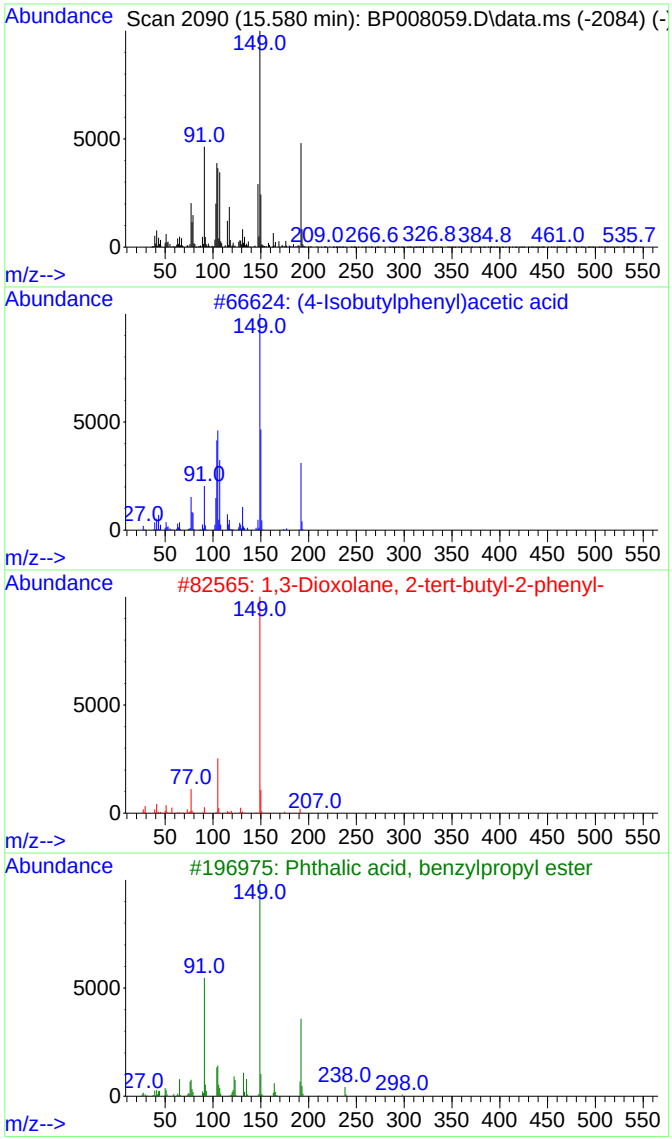
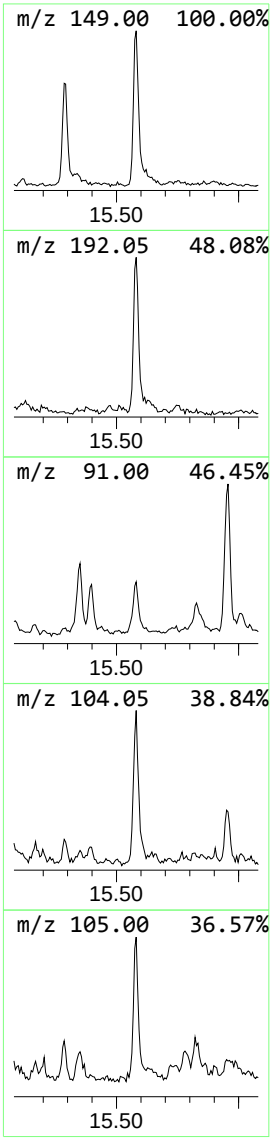
Peak Number 15 (4-Isobutylphenyl)acetic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.580	4.25 ng	309644	Acenaphthene-d10	14.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(4-Isobutylphenyl)acetic acid	192	C12H16O2	001553-60-2	74
2	1,3-Dioxolane, 2-tert-butyl-2-ph...	206	C13H18O2	006135-60-0	35
3	Phthalic acid, benzylpropyl ester	298	C18H18O4	1000309-04-2	32
4	Pyridine, 1-acetyl-5-(3,4-dihydr...	192	C11H16N2O	054966-57-3	32
5	Ethanol, 2-(4-phenoxyphenoxy)-, ...	334	C21H18O4	055191-59-8	27





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Data File : BP008059.D
Acq On : 20 Nov 2021 16:01
Operator : CG/JU
Sample : M4768-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-3

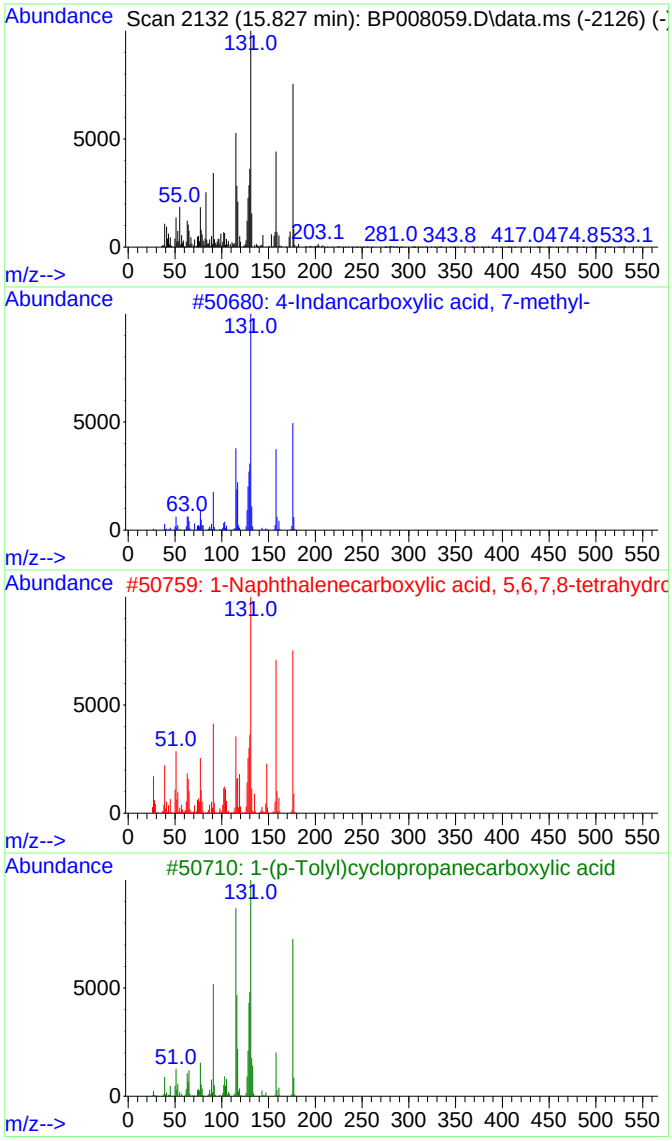
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

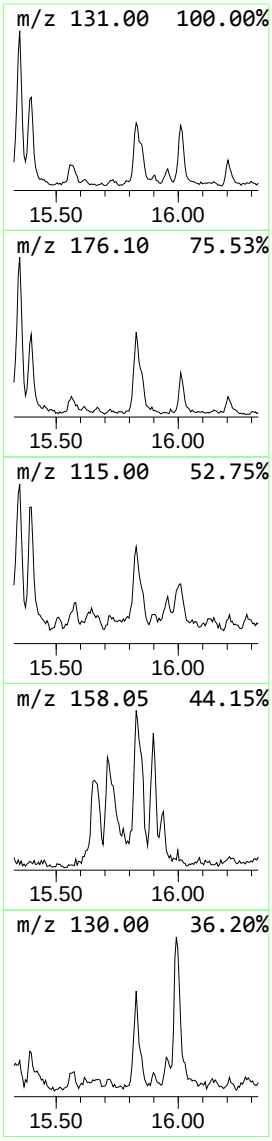
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 4-Indancarboxylic acid, 7-m... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.827	3.56 ng	259500	Acenaphthene-d10	14.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Indancarboxylic acid, 7-methyl-	176	C11H12O2	071042-74-5	98
2	1-Naphthalenecarboxylic acid, 5,...	176	C11H12O2	004242-18-6	94
3	1-(p-Tolyl)cyclopropanecarboxyli...	176	C11H12O2	083846-66-6	93
4	2-(1,2,3,4-Tetrahydronaphthalen-...	176	C12H16O	068480-12-6	87
5	(Indazol-1-yl)acetic acid	176	C9H8N2O2	1000315-94-2	41





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Data File : BP008059.D
Acq On : 20 Nov 2021 16:01
Operator : CG/JU
Sample : M4768-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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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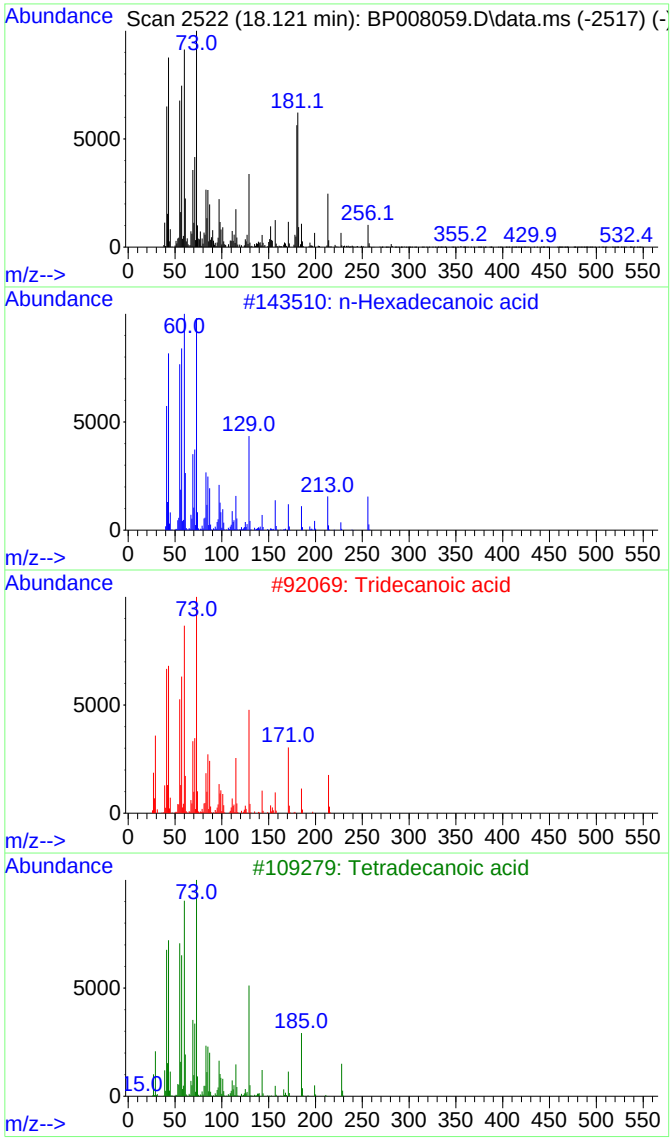
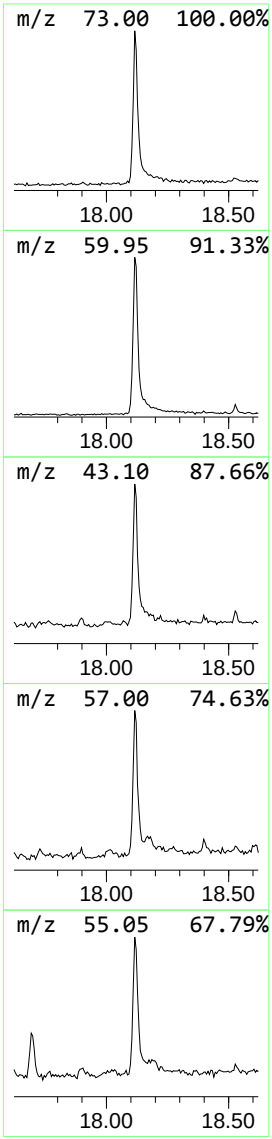
Peak Number 17 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.121	9.07 ng	732093	Phenanthrene-d10	17.215

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	96
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	Octadecanoic acid	284	C18H36O2	000057-11-4	64





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Data File : BP008059.D
Acq On : 20 Nov 2021 16:01
Operator : CG/JU
Sample : M4768-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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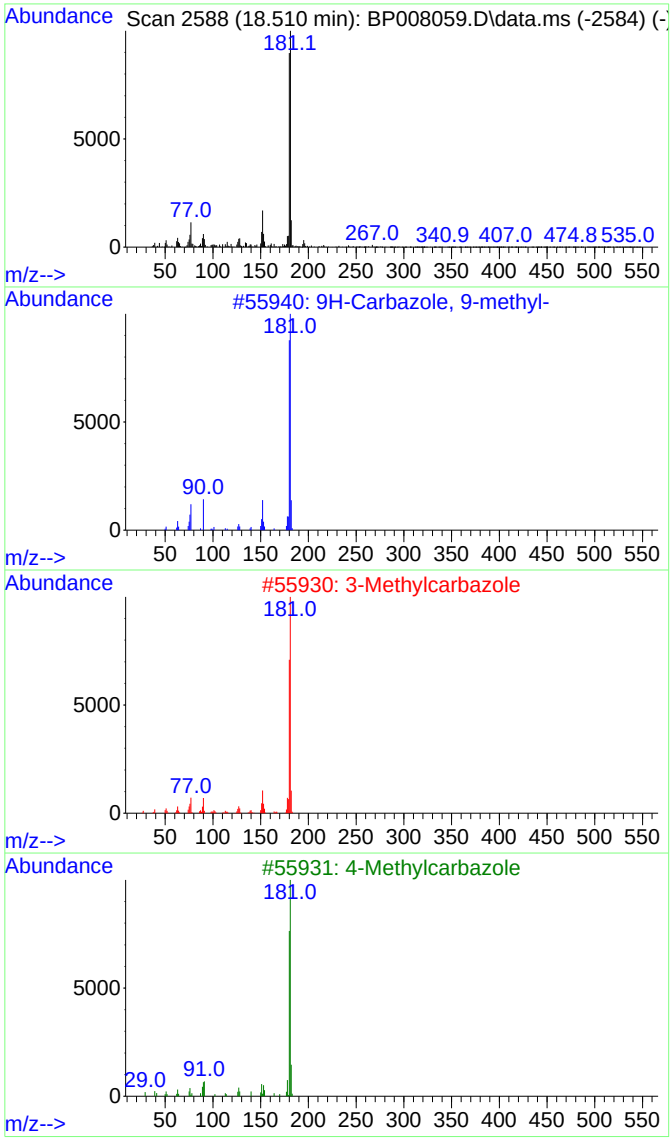
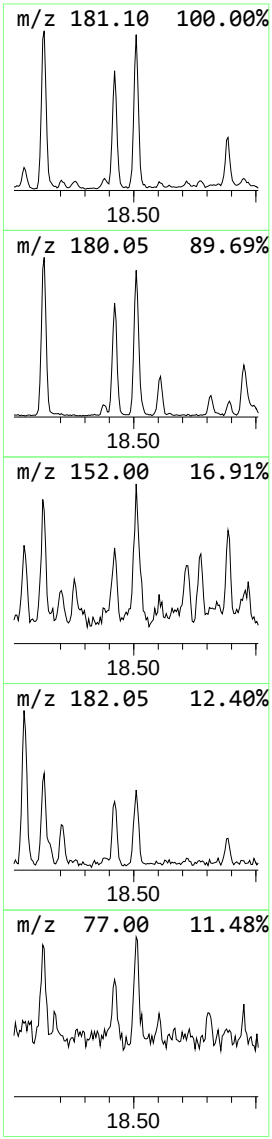
Peak Number 18 9H-Carbazole, 9-methyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.510	3.25 ng	262204	Phenanthrene-d10	17.215

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Carbazole, 9-methyl-	181	C13H11N	001484-12-4	94
2	3-Methylcarbazole	181	C13H11N	004630-20-0	93
3	4-Methylcarbazole	181	C13H11N	003770-48-7	93
4	Pyridine, 4-(2-phenylethenyl)-	181	C13H11N	000103-31-1	91
5	2-Fluorenamine	181	C13H11N	000153-78-6	90





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Operator : CG/JU
Sample : M4768-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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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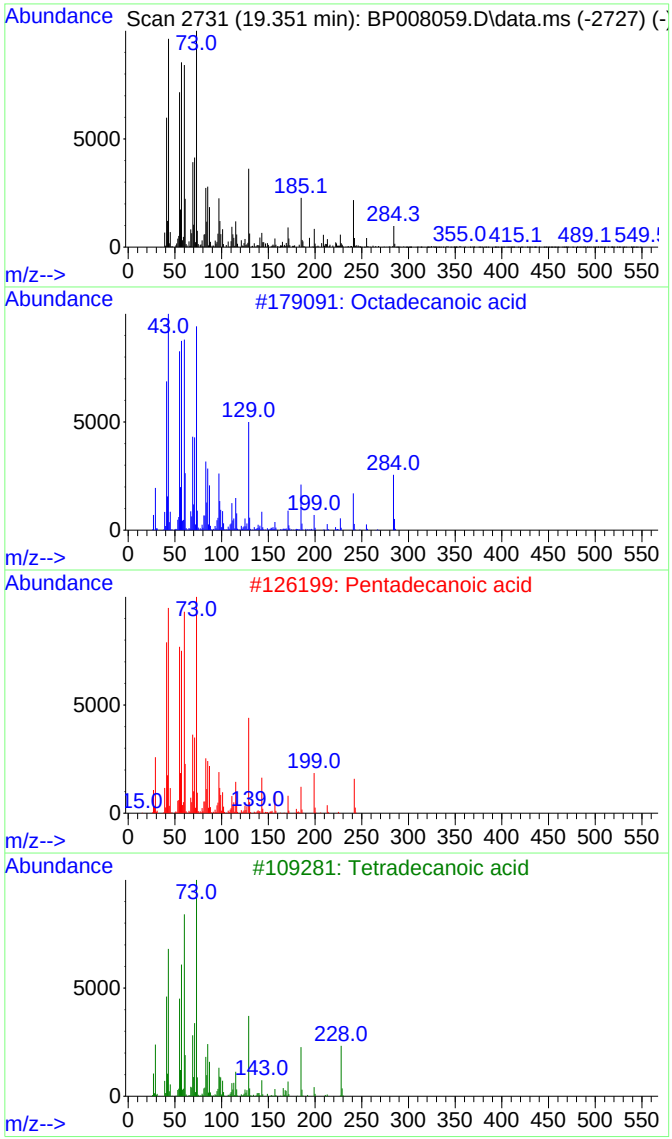
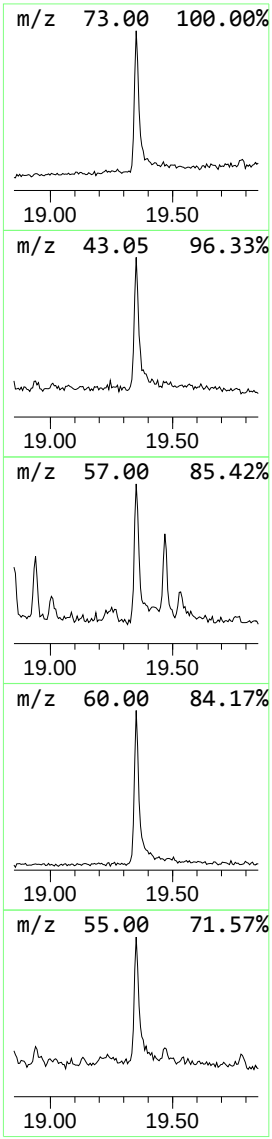
Peak Number 19 Octadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.351	3.91 ng	387372	Chrysene-d12	21.309

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64





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Data File : BP008059.D
Acq On : 20 Nov 2021 16:01
Operator : CG/JU
Sample : M4768-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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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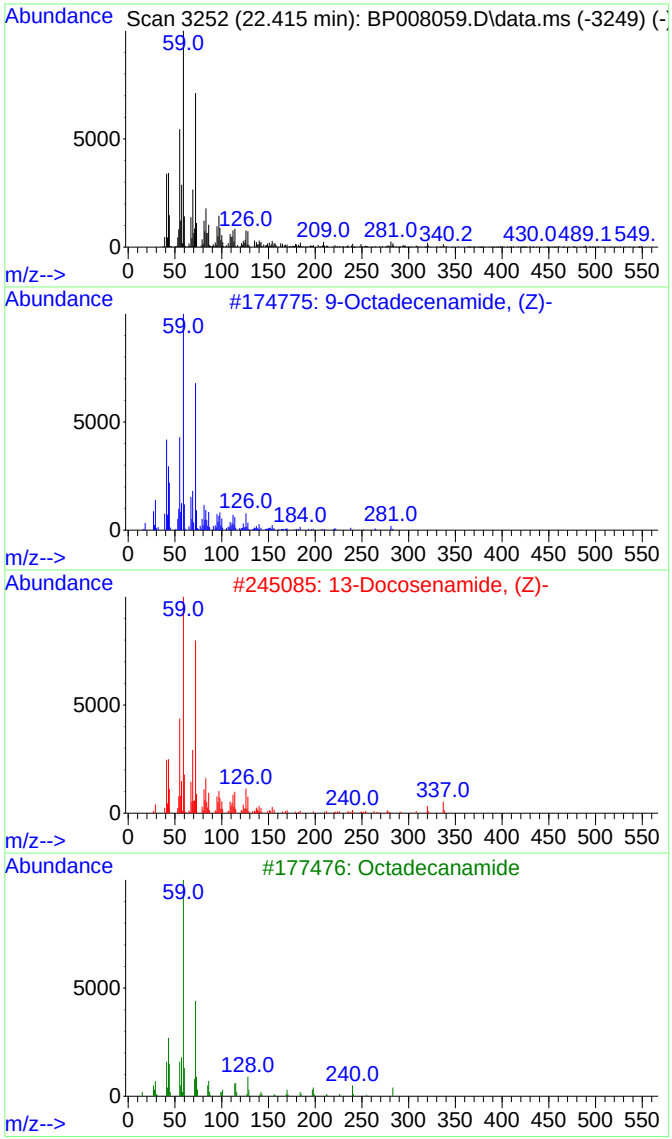
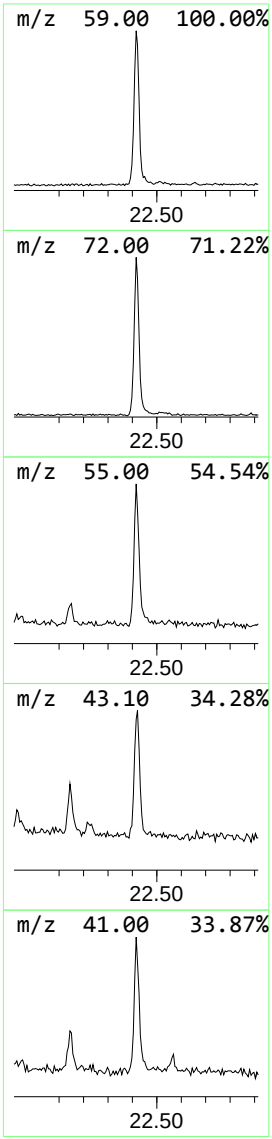
Peak Number 20 9-Octadecenamide, (Z)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.415	4.18 ng	414713	Chrysene-d12	21.309

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	78
3	Octadecanamide	283	C18H37NO	000124-26-5	72
4	Nonanamide	157	C9H19NO	001120-07-6	53
5	Palmitoleamide	253	C16H31NO	106010-22-4	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112021\
Data File : BP008059.D
Acq On : 20 Nov 2021 16:01
Operator : CG/JU
Sample : M4768-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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
Benzene, 1,3-di...	5.469	3.6	ng	140127	1	7.822	775027	20.0
Indane	8.192	7.4	ng	286001	1	7.822	775027	20.0
Benzene, 2-ethe...	10.022	6.0	ng	331870	2	10.616	1110370	20.0
2,2-Dimethylind...	10.675	4.1	ng	229595	2	10.616	1110370	20.0
Benzene, 1-meth...	10.739	3.9	ng	216774	2	10.616	1110370	20.0
Naphthalene, 1,...	11.086	5.6	ng	310662	2	10.616	1110370	20.0
Naphthalene, 1,...	11.204	6.4	ng	356343	2	10.616	1110370	20.0
Naphthalene, 1,...	12.175	3.5	ng	193901	2	10.616	1110370	20.0
2,5-Dimethylphe...	13.663	3.7	ng	271689	3	14.463	1458250	20.0
Benzoic acid, 2...	14.527	4.3	ng	310236	3	14.463	1458250	20.0
Phenylpropanamide	14.616	8.6	ng	624798	3	14.463	1458250	20.0
unknown15.080	15.080	4.6	ng	336902	3	14.463	1458250	20.0
3-Pentenoic aci...	15.351	5.8	ng	421058	3	14.463	1458250	20.0
2,3-Dihydro-1H-...	15.398	4.0	ng	295380	3	14.463	1458250	20.0
(4-Isobutylphen...	15.580	4.3	ng	309644	3	14.463	1458250	20.0
4-Indancarboxyl...	15.827	3.6	ng	259500	3	14.463	1458250	20.0
n-Hexadecanoic ...	18.121	9.1	ng	732093	4	17.215	1614330	20.0
9H-Carbazole, 9...	18.510	3.3	ng	262204	4	17.215	1614330	20.0
Octadecanoic acid	19.351	3.9	ng	387372	5	21.309	1983570	20.0
9-Octadecenamid...	22.415	4.2	ng	414713	5	21.309	1983570	20.0