LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112321\
Data File : BP008109.D
Acq On : 23 Nov 2021 22:25
Operator : CG/JU
Sample : M4803-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
266

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: BP008109.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	172	176	187	rVB	26083	43806	1.92%	0.113%
2	5.411	405	412	418	rBV	45785	69564	3.05%	0.180%
3	5.469	418	422	433	rVB2	20512	45024	1.97%	0.117%
4	5.846	480	486	493	rVB2	128917	193065	8.46%	0.500%
5	5.911	493	497	509	rVB	44100	73147	3.21%	0.189%
6	6.105	520	530	538	rBV4	28383	76686	3.36%	0.198%
7	6.222	544	550	556	rVB2	23946	46931	2.06%	0.121%
8	6.316	561	566	573	rVB4	29006	47363	2.08%	0.123%
9	6.387	573	578	583	rBV	40417	59410	2.60%	0.154%
10	6.463	587	591	603	rVB5	37574	83349	3.65%	0.216%
11	6.787	640	646	648	rBV2	32683	47346	2.07%	0.123%
12	6.822	648	652	657	rVV	68797	98048	4.30%	0.254%
13	6.875	657	661	665	rVV	78130	110854	4.86%	0.287%
14	6.987	673	680	688	rBV3	86546	169873	7.44%	0.440%
15	7.452	753	759	769	rBV2	303393	476849	20.90%	1.234%
16	7.822	814	822	830	rVB	546990	920496	40.34%	2.382%
17	8.016	851	855	860	rBV2	32320	48891	2.14%	0.127%
18	8.110	864	871	877	rVB4	27768	60678	2.66%	0.157%
19	8.357	906	913	920	rBV2	42638	70971	3.11%	0.184%
20	8.416	920	923	927	rBV	35294	45491	1.99%	0.118%
21	8.487	932	935	947	rVB	52956	93468	4.10%	0.242%
22	8.593	947	953	958	rBV	52264	88959	3.90%	0.230%
23	8.910	1000	1007	1017	rBV2	61286	155921	6.83%	0.403%
24	8.999	1017	1022	1026	rVV2	32303	74654	3.27%	0.193%
25	9.057	1027	1032	1042	rVB	224229	338563	14.84%	0.876%
26	9.540	1112	1114	1121	rVB5	29376	43864	1.92%	0.113%
27	9.704	1135	1142	1147	rBV5	19314	49070	2.15%	0.127%
28	9.804	1154	1159	1163	rBV6	23728	45456	1.99%	0.118%
29	9.904	1173	1176	1181	rVB	42747	69007	3.02%	0.179%
30	9.975	1184	1188	1193	rVB2	38416	53755	2.36%	0.139%
31	10.057	1198	1202	1210	rVB	63370	108481	4.75%	0.281%
32	10.163	1212	1220	1227	rBV3	58662	142739	6.26%	0.369%
33	10.616	1288	1297	1309	rBV2	900446	1886411	82.67%	4.881%
34	10.751	1315	1320	1323	rBV5	35562	55788	2.44%	0.144%
35	10.793	1323	1327	1333	rVV	105061	160439	7.03%	0.415%
36	10.857	1334	1338	1345	rVV3	46675	91083	3.99%	0.236%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112321\
Data File : BP008109.D
Acq On : 23 Nov 2021 22:25
Operator : CG/JU
Sample : M4803-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
266

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	10.922	1345	1349	1356	rVB4	29234	53594	2.35%	0.139%
38	11.028	1361	1367	1374	rVB4	32051	68074	2.98%	0.176%
39	11.116	1377	1382	1386	rVV4	27389	44271	1.94%	0.115%
40	11.193	1387	1395	1402	rVB8	35314	89019	3.90%	0.230%
41	11.328	1408	1418	1421	rBV6	73994	164417	7.21%	0.425%
42	11.363	1421	1424	1427	rVV	61800	94783	4.15%	0.245%
43	11.393	1427	1429	1436	rVB	88470	129770	5.69%	0.336%
44	11.469	1437	1442	1449	rVB	90567	142492	6.24%	0.369%
45	11.551	1449	1456	1464	rVB	162193	292480	12.82%	0.757%
46	11.657	1464	1474	1479	rBV	229211	440637	19.31%	1.140%
47	11.869	1505	1510	1514	rBV	104042	151158	6.62%	0.391%
48	12.057	1536	1542	1547	rBV	845587	1207042	52.90%	3.123%
49	12.334	1585	1589	1594	rBV6	27779	65498	2.87%	0.169%
50	12.422	1599	1604	1612	rVB3	82371	152374	6.68%	0.394%
51	12.504	1613	1618	1621	rBV5	51388	97733	4.28%	0.253%
52	12.546	1622	1625	1629	rVB3	41052	65695	2.88%	0.170%
53	12.693	1646	1650	1653	rBV	62215	77392	3.39%	0.200%
54	12.734	1653	1657	1662	rBV3	53637	110518	4.84%	0.286%
55	12.804	1662	1669	1673	rBV2	160601	278867	12.22%	0.722%
56	12.893	1677	1684	1691	rVB3	176665	370081	16.22%	0.958%
57	12.957	1692	1695	1697	rBV2	66104	87237	3.82%	0.226%
58	13.051	1707	1711	1715	rBV3	93725	131216	5.75%	0.340%
59	13.257	1741	1746	1750	rBV	362223	517880	22.70%	1.340%
60	13.298	1750	1753	1759	rVB	396183	499245	21.88%	1.292%
61	13.422	1771	1774	1778	rVB	61259	78085	3.42%	0.202%
62	13.528	1784	1792	1798	rVB	354155	680725	29.83%	1.761%
63	13.616	1803	1807	1813	rVV	141844	210472	9.22%	0.545%
64	13.675	1815	1817	1823	rVB2	46115	56355	2.47%	0.146%
65	13.728	1823	1826	1829	rBV3	35611	49005	2.15%	0.127%
66	13.940	1858	1862	1863	rBV3	69021	88081	3.86%	0.228%
67	14.298	1920	1923	1930	rVB4	104269	192926	8.45%	0.499%
68	14.375	1932	1936	1940	rBV	100211	133256	5.84%	0.345%
69	14.428	1940	1945	1947	rBV	239250	339875	14.89%	0.879%
70	14.469	1947	1952	1956	rVV	1173140	1873280	82.10%	4.847%
71	14.504	1956	1958	1962	rVB2	262704	281188	12.32%	0.728%
72	14.645	1979	1982	1987	rVB	88630	105609	4.63%	0.273%
73	15.257	2082	2086	2090	rBV4	123602	180831	7.92%	0.468%
74	15.416	2109	2113	2120	rVB	332571	447400	19.61%	1.158%
75	16.139	2233	2236	2237	rBV	150542	162384	7.12%	0.420%
76	16.222	2247	2250	2253	rBV	179617	203742	8.93%	0.527%

LSC Area Percent Report

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Acq On : 23 Nov 2021 22:25
Operator : CG/JU
Sample : M4803-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
266

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	16.463	2287	2291	2301	rVB	534065	821977	36.02%	2.127%
78	16.622	2314	2318	2326	rVB	760758	998119	43.74%	2.583%
79	16.692	2326	2330	2334	rVB	264056	349684	15.32%	0.905%
80	17.045	2387	2390	2399	rVB3	261936	469599	20.58%	1.215%
81	17.228	2416	2421	2430	rBV	1408069	2281813	100.00%	5.904%
82	17.310	2431	2435	2441	rVB2	503718	775502	33.99%	2.007%
83	17.375	2443	2446	2453	rVB4	222772	375440	16.45%	0.971%
84	17.622	2485	2488	2492	rVB2	240539	314590	13.79%	0.814%
85	17.892	2531	2534	2536	rBV2	276380	358887	15.73%	0.929%
86	18.022	2550	2556	2560	rBV2	549750	1222733	53.59%	3.164%
87	18.863	2696	2699	2703	rVB	525444	564721	24.75%	1.461%
88	18.945	2710	2713	2719	rVB	847281	1063791	46.62%	2.753%
89	19.480	2800	2804	2807	rBV	478733	573075	25.11%	1.483%
90	19.998	2889	2892	2896	rVB	628312	718686	31.50%	1.860%
91	20.469	2969	2972	2979	rVB	631406	824224	36.12%	2.133%
92	20.669	3003	3006	3009	rVB	562975	577010	25.29%	1.493%
93	20.716	3011	3014	3017	rBV	878743	944854	41.41%	2.445%
94	20.780	3022	3025	3032	rVB	467711	696785	30.54%	1.803%
95	21.157	3085	3089	3090	rBV2	1257197	1596846	69.98%	4.132%
96	21.322	3113	3117	3124	rBV	1441938	1999484	87.63%	5.174%
97	21.586	3159	3162	3166	rBV	591949	785425	34.42%	2.032%
98	22.051	3238	3241	3248	rVB	560018	702775	30.80%	1.818%
99	22.304	3281	3284	3289	rVB	731534	967207	42.39%	2.503%
100	23.727	3522	3526	3533	rVB2	1048346	2003438	87.80%	5.184%

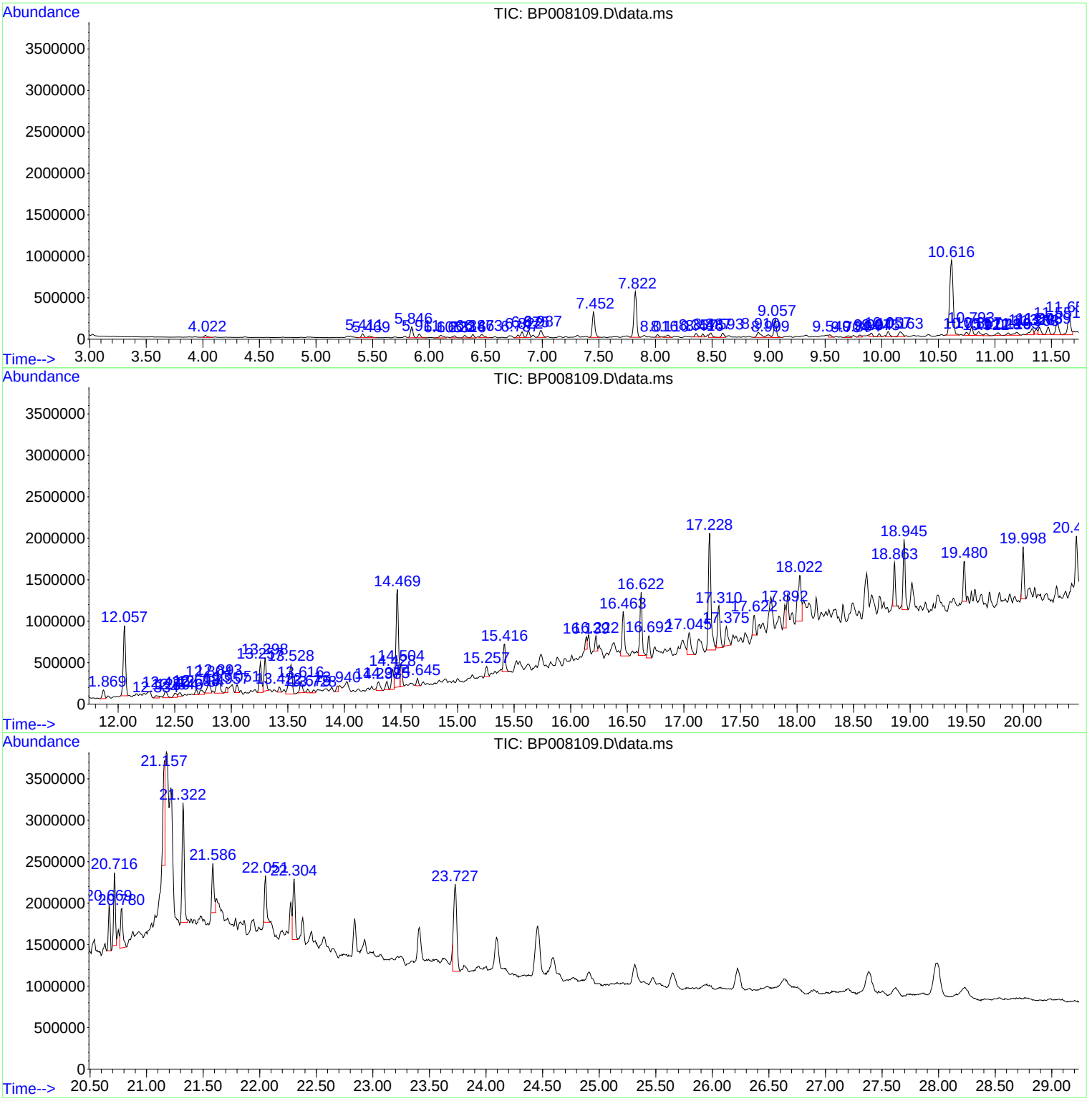
Sum of corrected areas: 38646852

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112321\
Data File : BP008109.D
Acq On : 23 Nov 2021 22:25
Operator : CG/JU
Sample : M4803-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
266

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\BP112321\
Data File : BP008109.D
Acq On : 23 Nov 2021 22:25
Operator : CG/JU
Sample : M4803-01 10X
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ALS Vial : 17 Sample Multiplier: 1

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

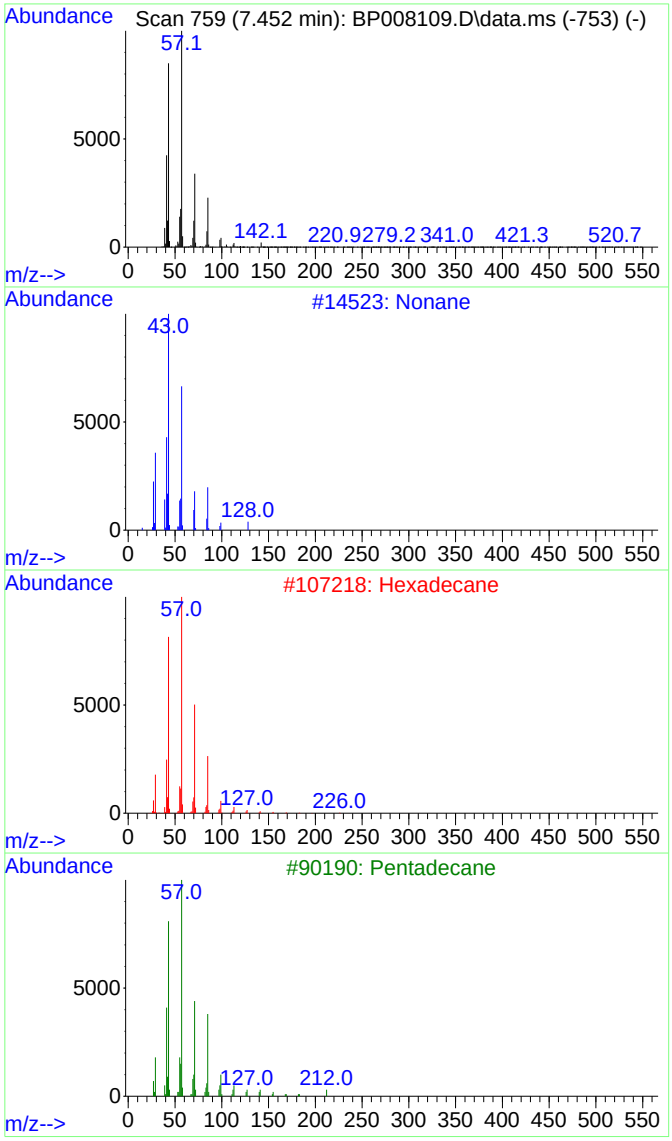
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

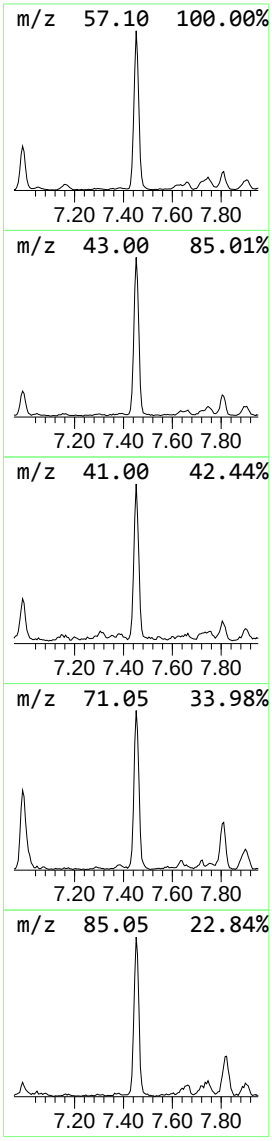
****

Peak Number 1 Nonane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.452	10.36 ng	476849	1,4-Dichlorobenzene-d4	7.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane	128	C9H20	000111-84-2	90
2	Hexadecane	226	C16H34	000544-76-3	78
3	Pentadecane	212	C15H32	000629-62-9	78
4	Tridecane	184	C13H28	000629-50-5	78
5	Undecane	156	C11H24	001120-21-4	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112321\
Data File : BP008109.D
Acq On : 23 Nov 2021 22:25
Operator : CG/JU
Sample : M4803-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
266

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

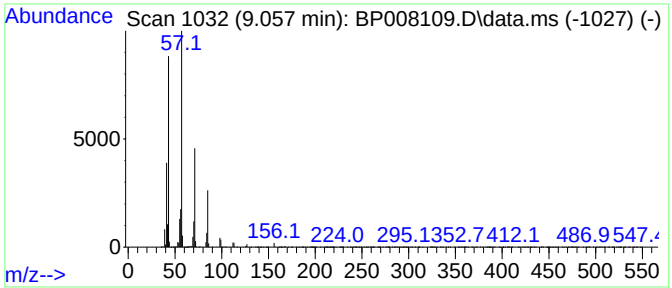
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

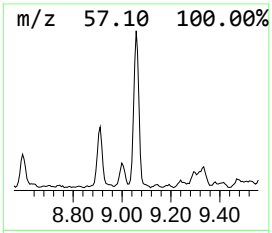
****

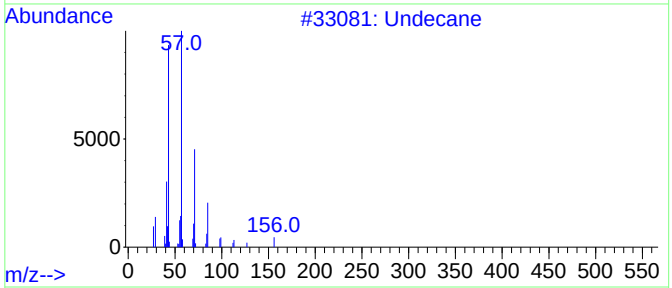
Peak Number 2 Undecane Concentration Rank 11

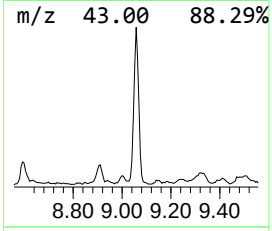
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.057	7.36 ng	338563	1,4-Dichlorobenzene-d4	7.822

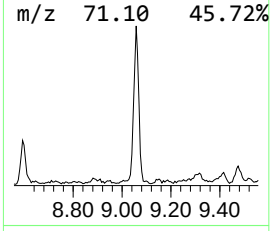
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	91
2	Hexatriacontane	507	C36H74	000630-06-8	86
3	Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	83
4	Tridecane	184	C13H28	000629-50-5	83
5	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	80

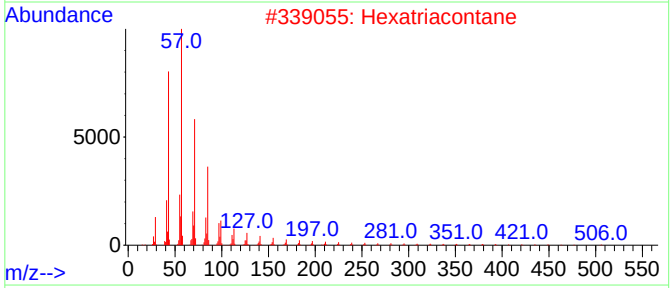


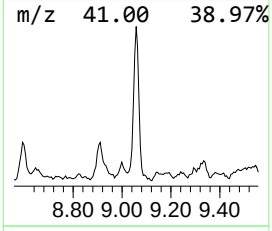


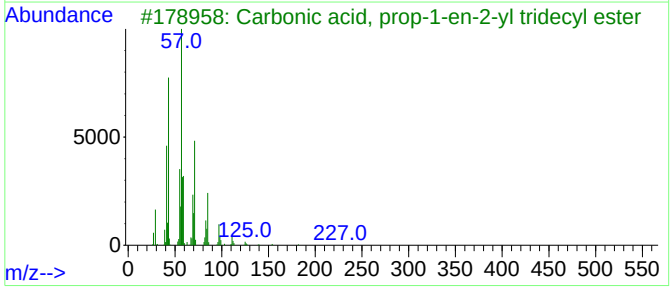


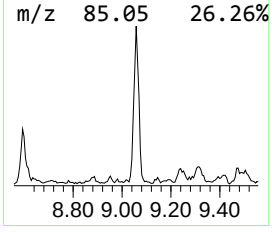












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112321\
Data File : BP008109.D
Acq On : 23 Nov 2021 22:25
Operator : CG/JU
Sample : M4803-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
266

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

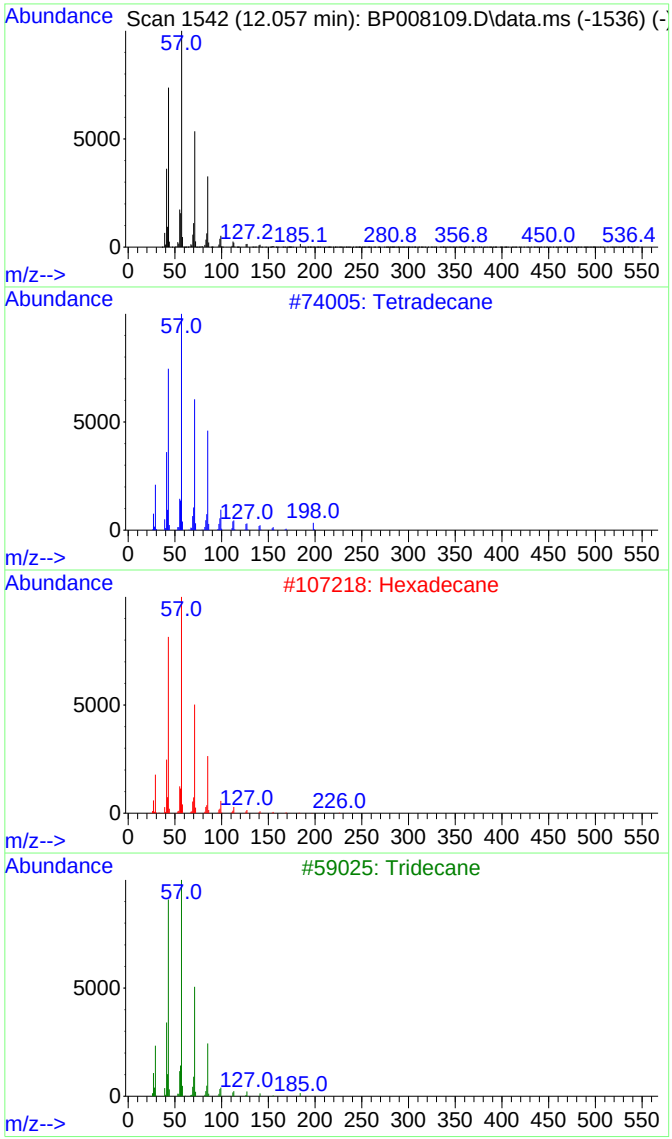
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

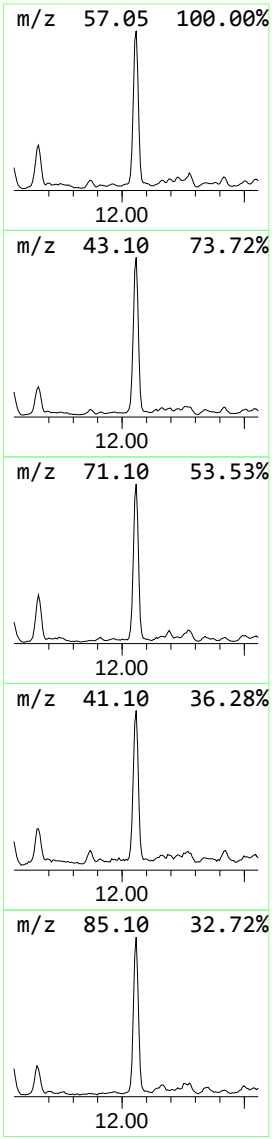
****

Peak Number 3 Tetradecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.057	12.80 ng	1207040	Naphthalene-d8	10.622

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tridecane	184	C13H28	000629-50-5	76
4	Pentadecane	212	C15H32	000629-62-9	59
5	Undecane	156	C11H24	001120-21-4	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112321\
Data File : BP008109.D
Acq On : 23 Nov 2021 22:25
Operator : CG/JU
Sample : M4803-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

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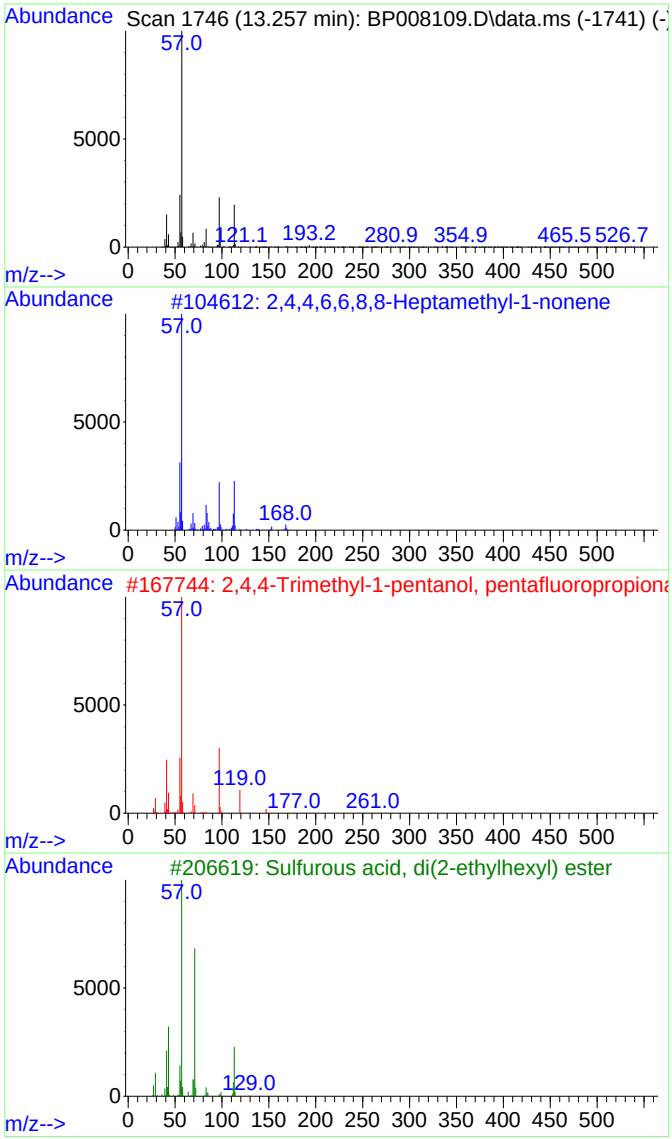
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

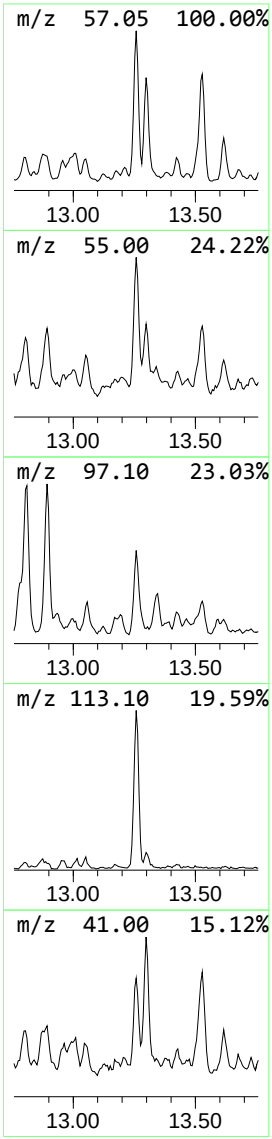
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.257	5.53 ng	517880	Acenaphthene-d10	14.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	72
2	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	38
3	Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	38
4	Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	33
5	2,4,4-Trimethyl-1-pentanol, chlo...	242	C10H17ClF2O2	1000447-27-2	32





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Data File : BP008109.D
Acq On : 23 Nov 2021 22:25
Operator : CG/JU
Sample : M4803-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
266

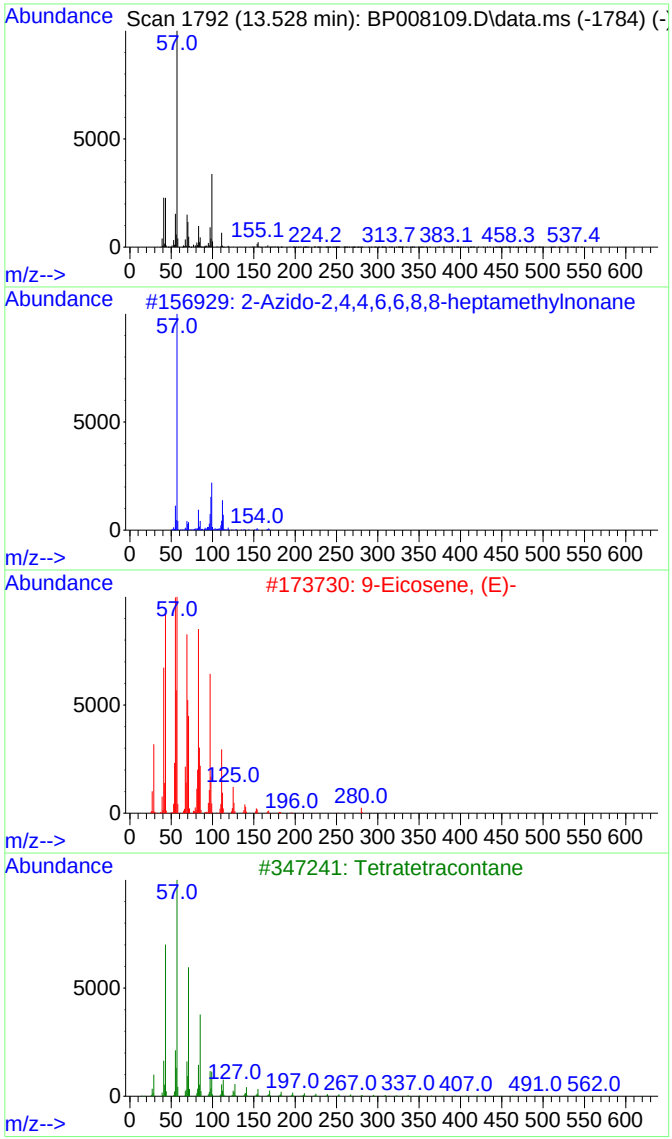
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

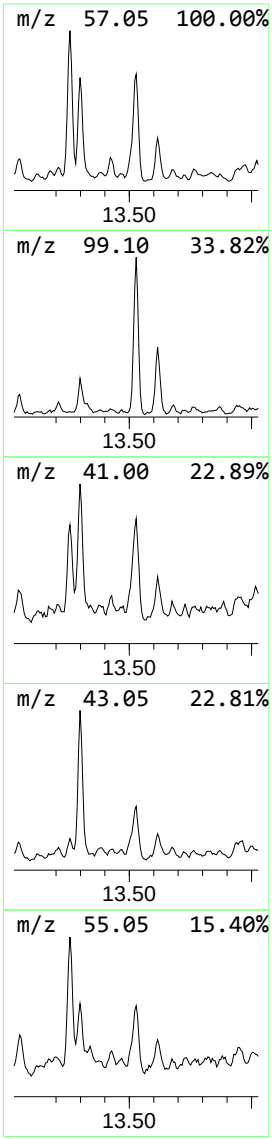
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Azido-2,4,4,6,6,8,8-hepta... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.528	7.27 ng	680725	Acenaphthene-d10	14.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Azido-2,4,4,6,6,8,8-heptamethy...	267	C16H33N3	1000293-29-1	59
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	47
3	Tetratetracontane	619	C44H90	007098-22-8	45
4	4-Propionyloxytetradecane	270	C17H34O2	1000245-62-9	45
5	Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	42





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Acq On : 23 Nov 2021 22:25
Operator : CG/JU
Sample : M4803-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

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

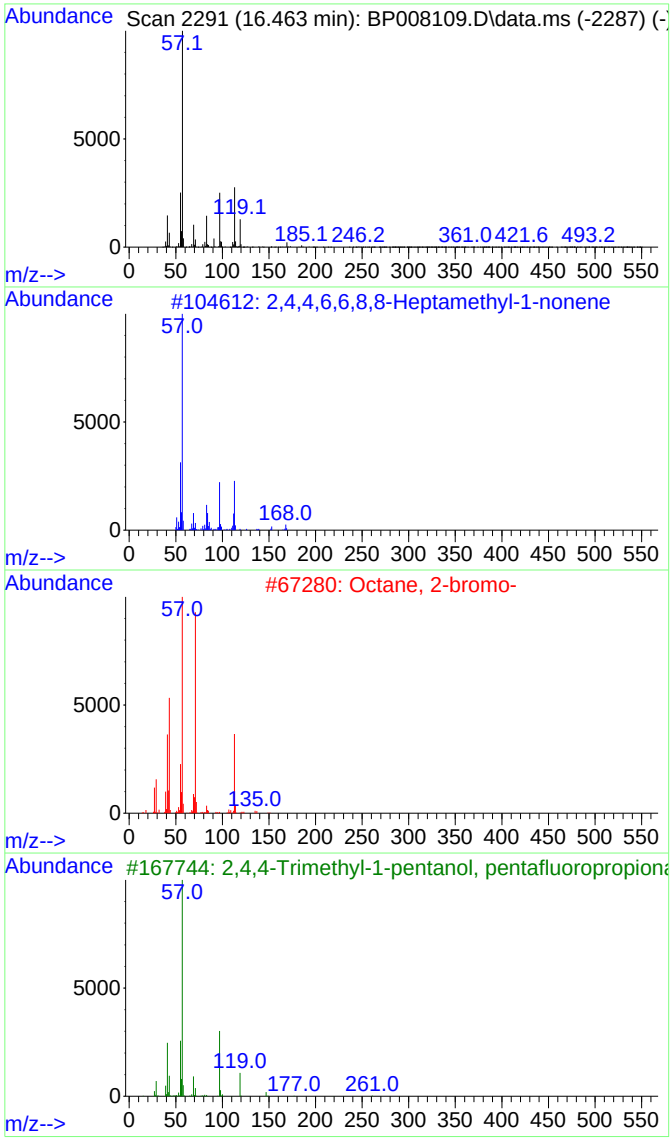
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

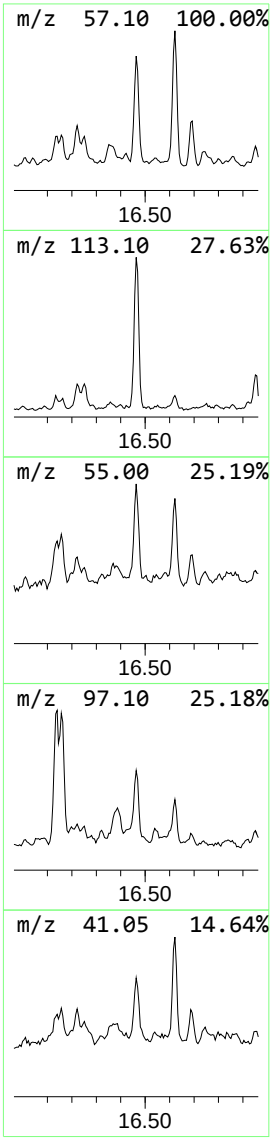
****

Peak Number 6 unknown16.463 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.463	7.20 ng	821977	Phenanthrene-d10	17.228

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	64
2	Octane, 2-bromo-	192	C8H17Br	000557-35-7	43
3	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	38
4	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	38
5	2,4,4-Trimethyl-1-pentanol, chlo...	242	C10H17ClF2O2	1000447-27-2	32





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Operator : CG/JU
Sample : M4803-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

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

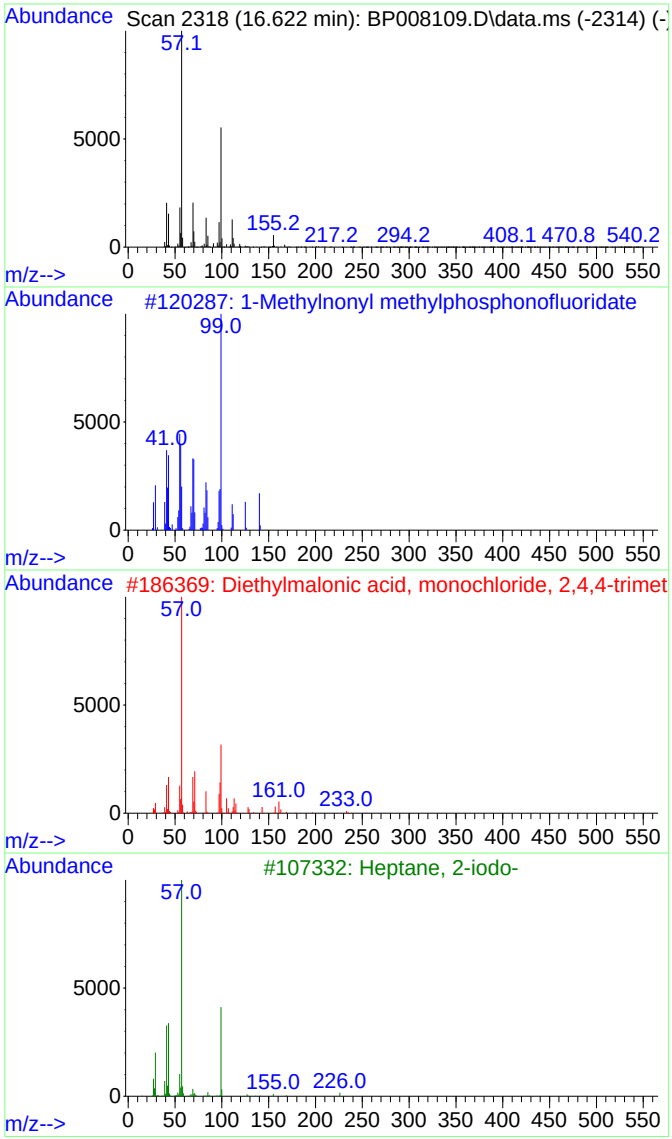
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

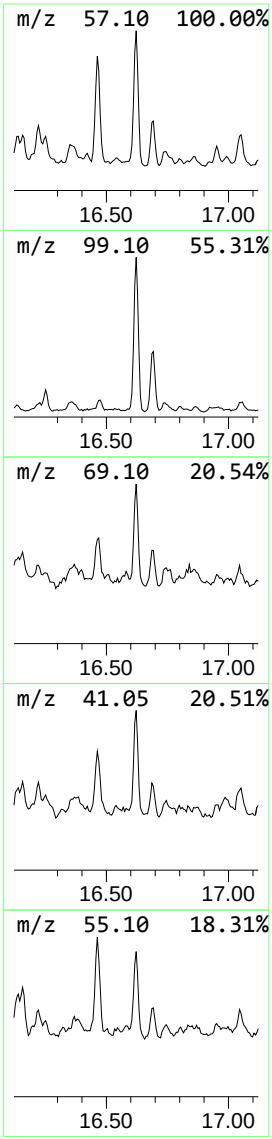
****

Peak Number 7 1-Methylnonyl methylphospho... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.622	8.75 ng	998119	Phenanthrene-d10	17.228

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methylnonyl methylphosphonoflu...	238	C11H24FO2P	211192-71-1	53
2	Diethylmalonic acid, monochlorid...	290	C15H27ClO3	1010369-49-2	50
3	Heptane, 2-iodo-	226	C7H15I	018589-29-2	47
4	2-Azido-2,4,4,6,6,8,8-heptamethy...	267	C16H33N3	1000293-29-1	40
5	3,5,5-Trimethyl-1-hexyl methylph...	224	C10H22FO2P	1000298-44-9	40





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Acq On : 23 Nov 2021 22:25
Operator : CG/JU
Sample : M4803-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
266

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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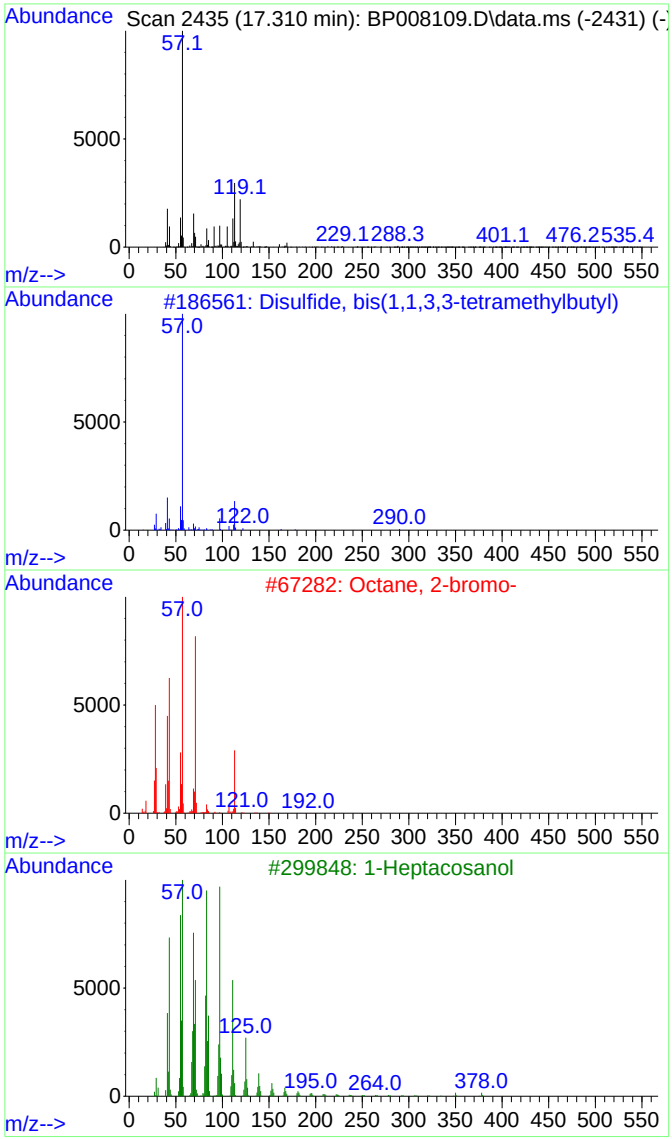
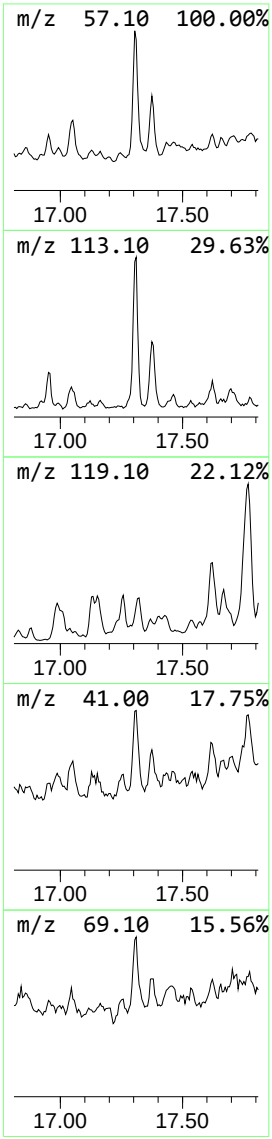
Peak Number 8 unknown17.310 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.310	6.80 ng	775502	Phenanthrene-d10	17.228

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, bis(1,1,3,3-tetrameth...	290	C16H34S2	029956-99-8	38
2	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35
3	1-Heptacosanol	396	C27H56O	002004-39-9	22
4	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	14
5	Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	12





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Acq On : 23 Nov 2021 22:25
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Misc :
ALS Vial : 17 Sample Multiplier: 1

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

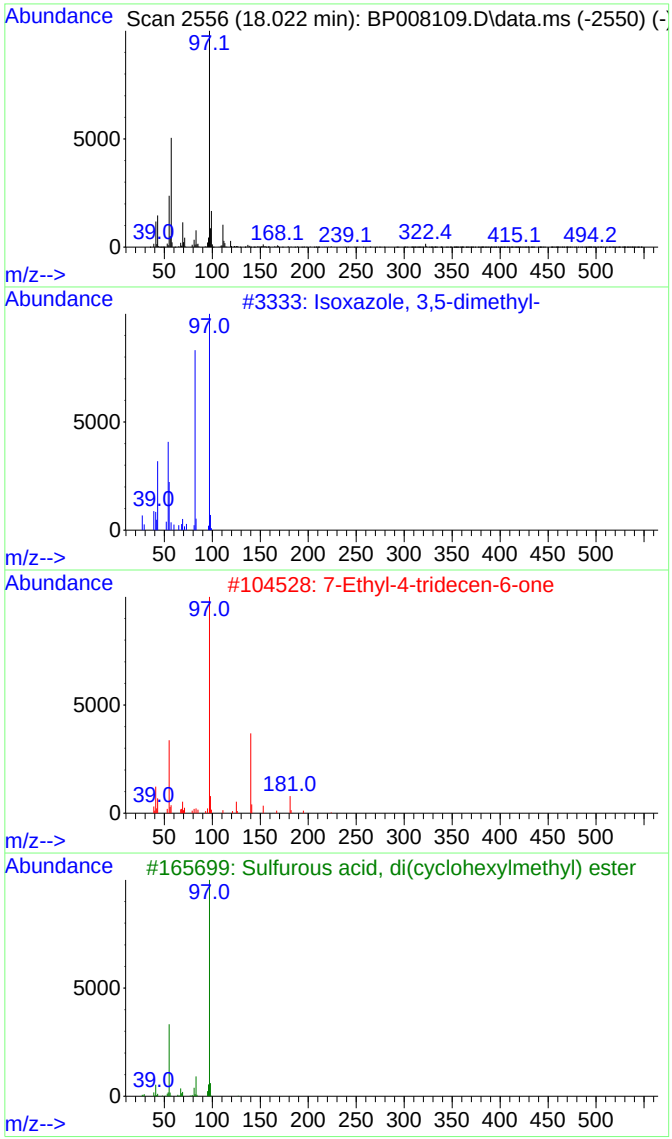
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

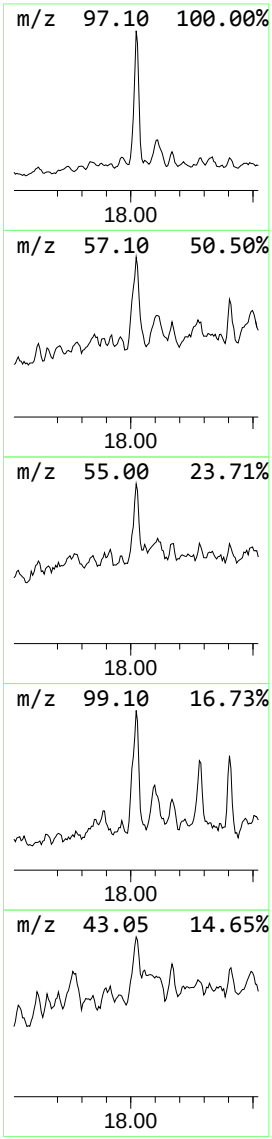
****

Peak Number 9 Isoxazole, 3,5-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.022	10.72 ng	1222730	Phenanthrene-d10	17.228

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	53
2	7-Ethyl-4-tridecen-6-one	224	C15H28O	1010374-07-1	53
3	Sulfurous acid, di(cyclohexylmet...	274	C14H26O3S	1010309-22-7	50
4	Cyclopentanecarboxylic acid, 4-h...	338	C22H42O2	1000282-77-5	45
5	Sulfurous acid, cyclohexylmethyl...	388	C22H44O3S	1000309-22-3	45





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Acq On : 23 Nov 2021 22:25
Operator : CG/JU
Sample : M4803-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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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

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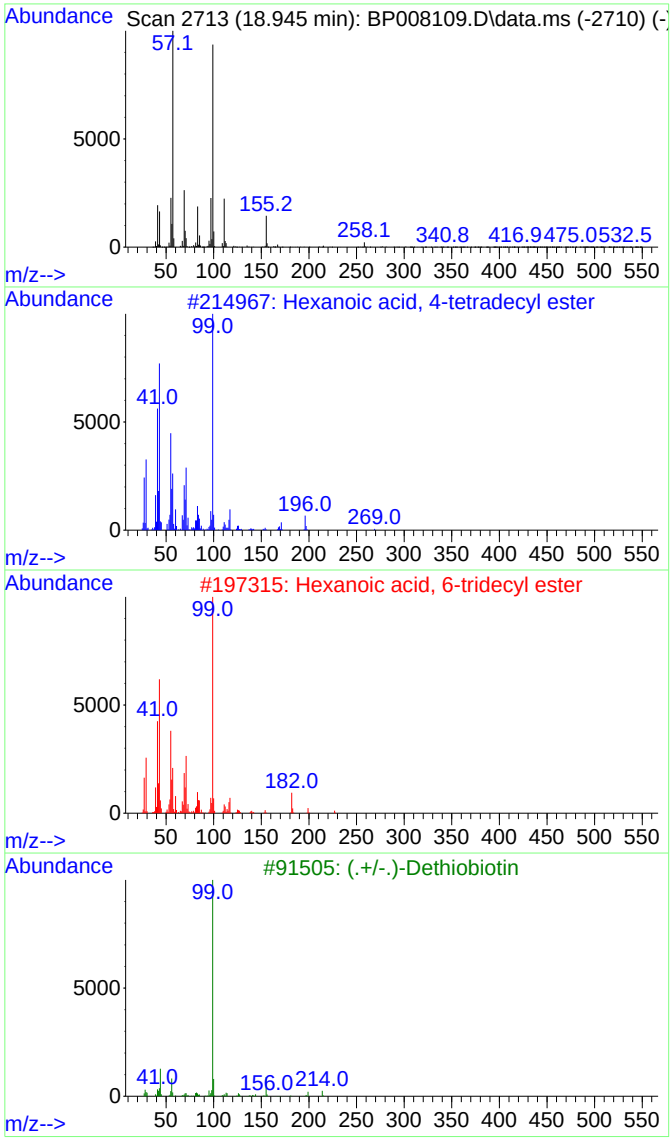
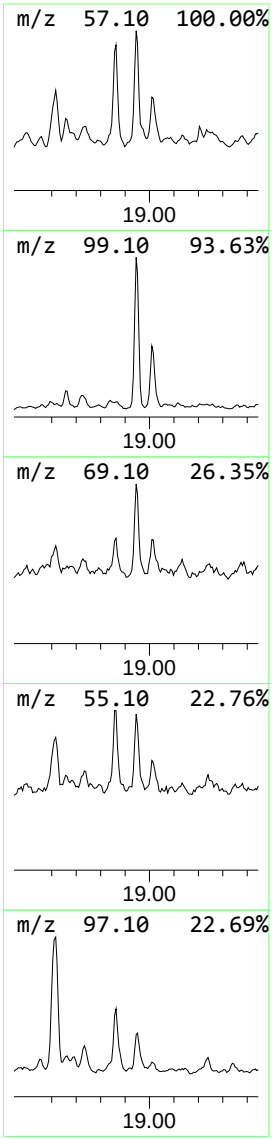
Peak Number 10 unknown18.945 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.945	9.32 ng	1063790	Phenanthrene-d10	17.228

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 4-tetradecyl ester	312	C20H40O2	1000279-29-8	47
2	Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	47
3	(.+/-.)-Dethiobiotin	214	C10H18N2O3	000636-20-4	47
4	Hexanoic acid, 4-tridecyl ester	298	C19H38O2	1000279-29-3	47
5	1-Pyrrolidinocarbonylmethyl pipe...	197	C10H19N3O	039890-45-4	47





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Acq On : 23 Nov 2021 22:25
Operator : CG/JU
Sample : M4803-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

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

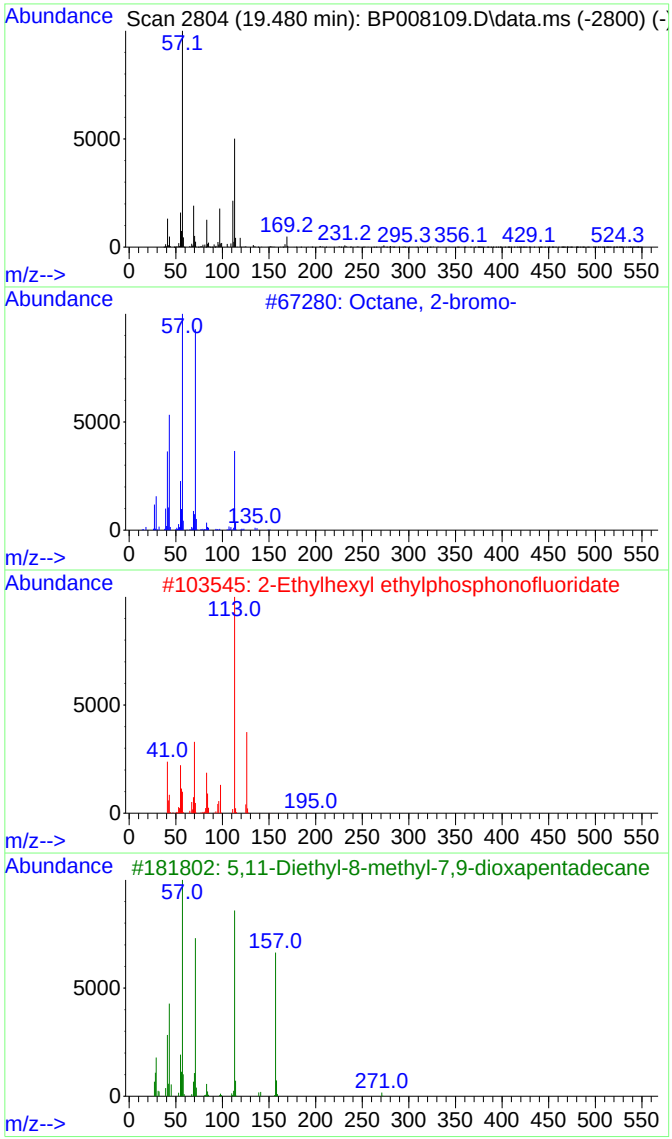
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

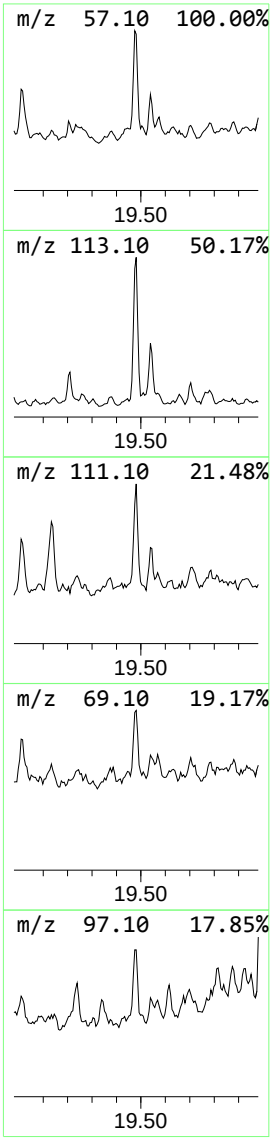
****

Peak Number 11 unknown19.480 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.480	5.73 ng	573075	Chrysene-d12	21.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-bromo-	192	C8H17Br	000557-35-7	37
2	2-Ethylhexyl ethylphosphonofluor...	224	C10H22FO2P	1000298-44-7	25
3	5,11-Diethyl-8-methyl-7,9-dioxap...	286	C18H38O2	1000334-83-1	25
4	Succinic acid, di(4-methylhept-3...	342	C20H38O4	1000467-92-2	23
5	3-Methylbutyl ethylphosphonofluo...	182	C7H16FO2P	1000273-49-8	22





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Acq On : 23 Nov 2021 22:25
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Sample : M4803-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

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

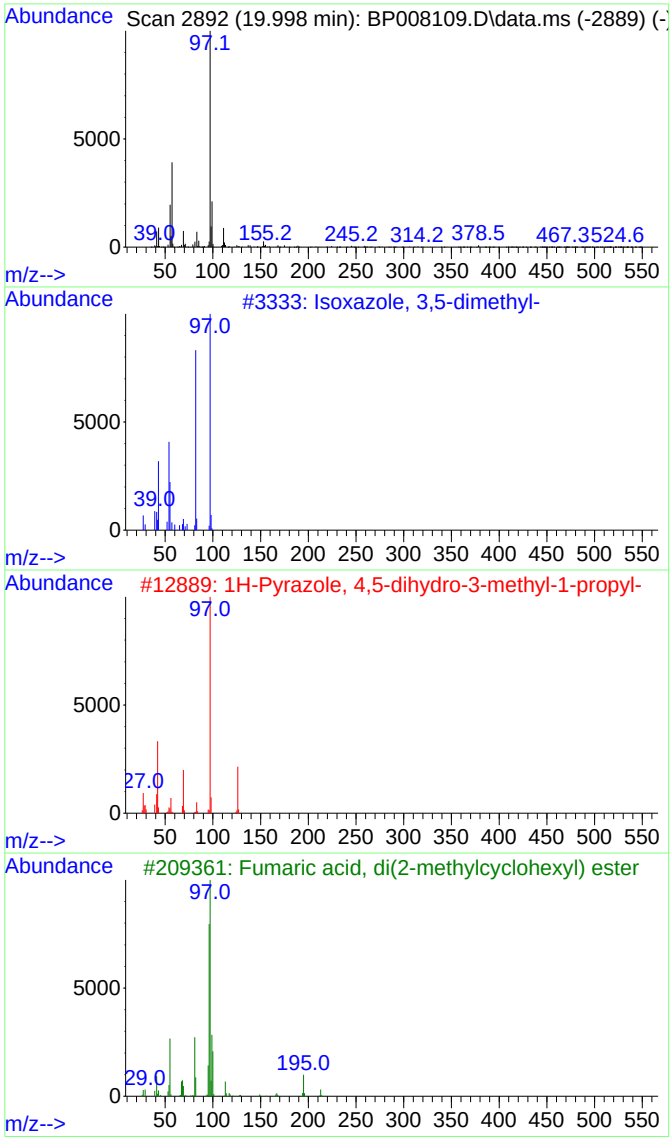
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

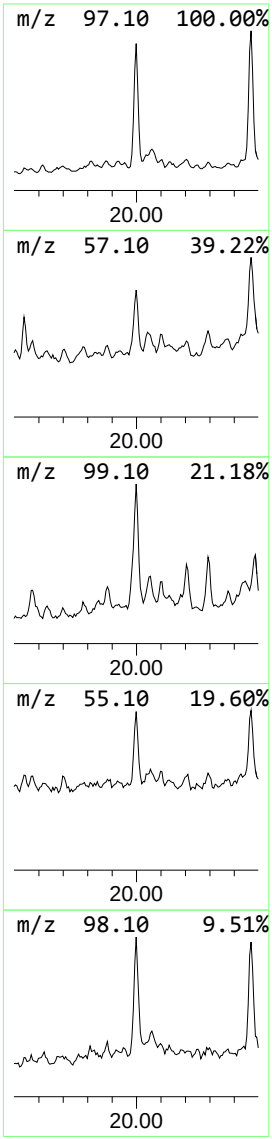
****

Peak Number 12 unknown19.998 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.998	7.19 ng	718686	Chrysene-d12	21.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	52
2	1H-Pyrazole, 4,5-dihydro-3-methy...	126	C7H14N2	026964-49-8	40
3	Fumaric acid, di(2-methylcyclohe...	308	C18H28O4	1000345-10-9	39
4	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1010309-21-6	38
5	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	38





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Sample : M4803-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

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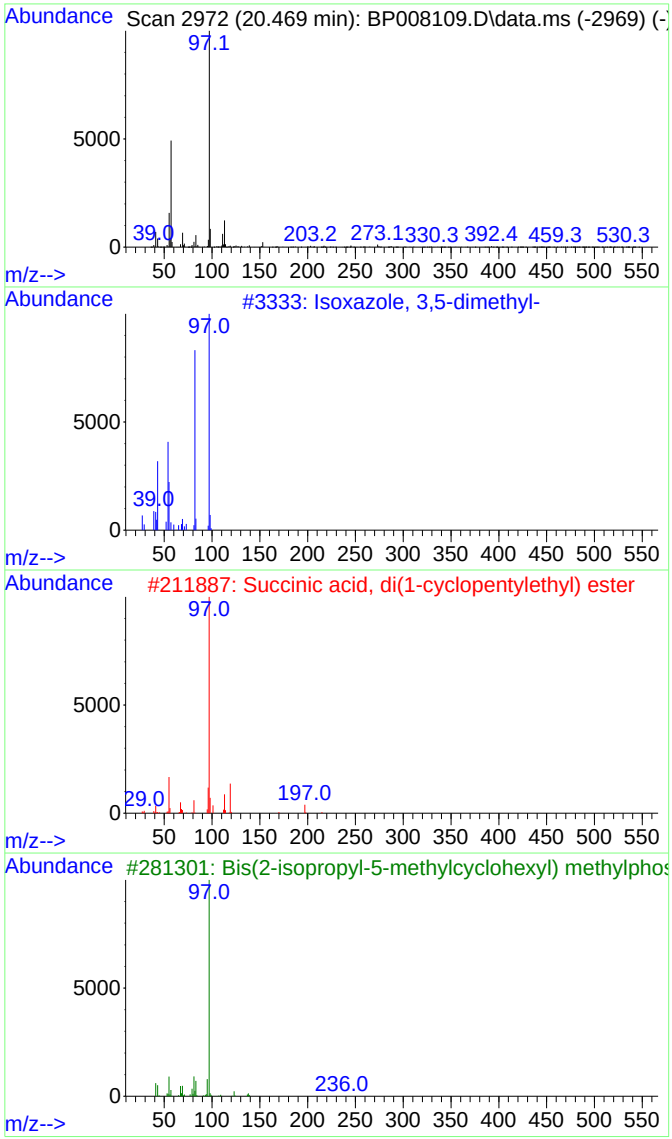
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

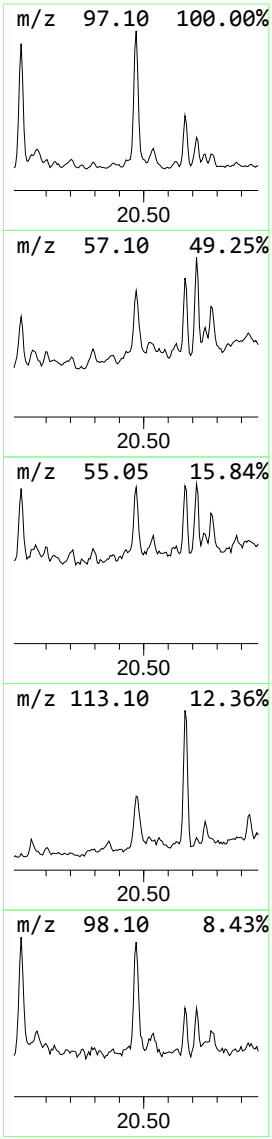
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Succinic acid, di(1-cyclope... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.469	8.24 ng	824224	Chrysene-d12	21.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	53
2	Succinic acid, di(1-cyclopentyle...	310	C18H30O4	1000330-21-8	50
3	Bis(2-isopropyl-5-methylcyclohex...	372	C21H41O3P	1000510-36-7	42
4	4-Methyl-2,3-hexadien-1-ol	112	C7H12O	1000196-09-6	42
5	Succinic acid, 2-methylpent-3-yl...	298	C17H30O4	1000391-41-0	39





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ALS Vial : 17 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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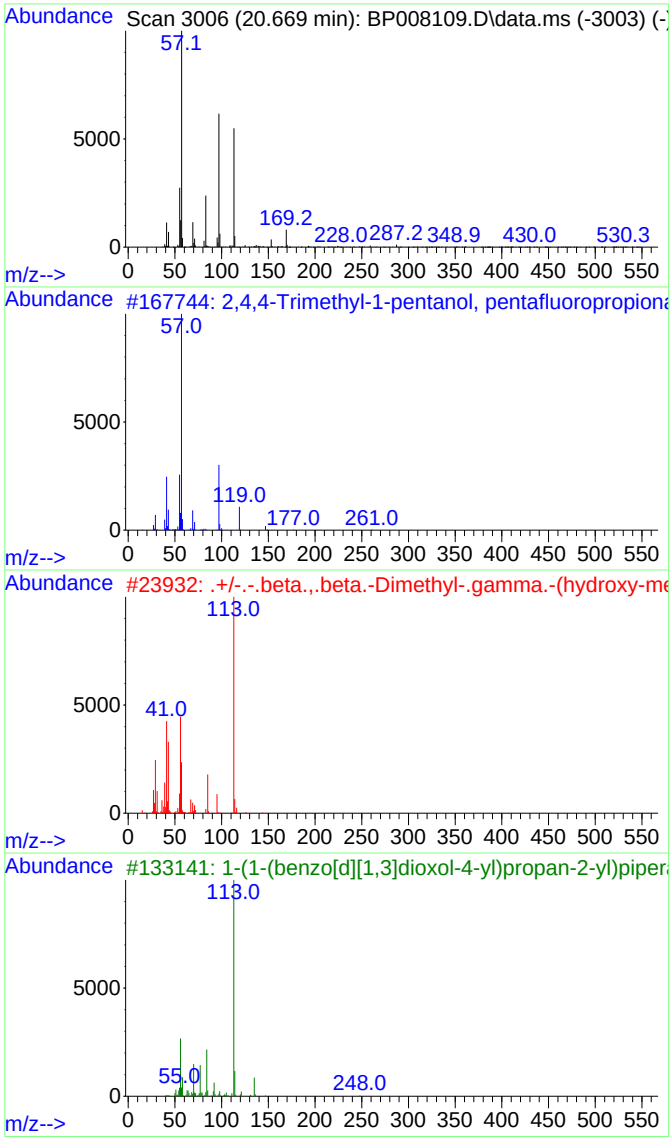
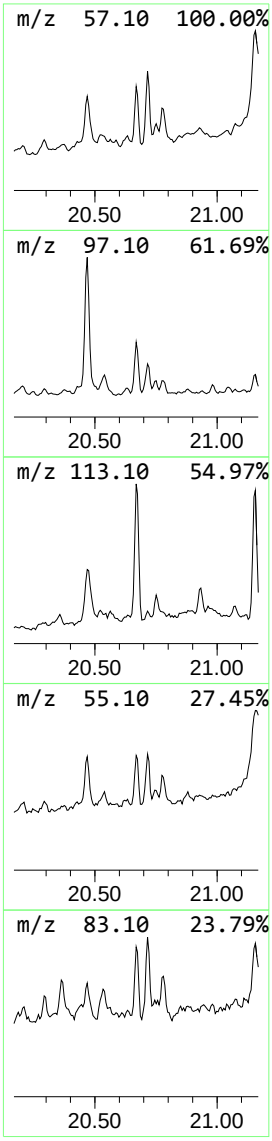
Peak Number 14 unknown20.669 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.669	5.77 ng	577010	Chrysene-d12	21.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	25
2	.+/-.-.beta.,.beta.-Dimethyl-.ga...	144	C7H12O3	052398-48-8	22
3	1-(1-(benzo[d][1,3]dioxol-4-yl)p...	248	C14H20N2O2	1000455-13-3	22
4	1-(2-methoxyphenyl)-2-(piperazin...	248	C14H20N2O2	1000455-13-6	18
5	2-Allylpent-4-enoic acid, methyl...	154	C9H14O2	054385-33-0	18





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ALS Vial : 17 Sample Multiplier: 1

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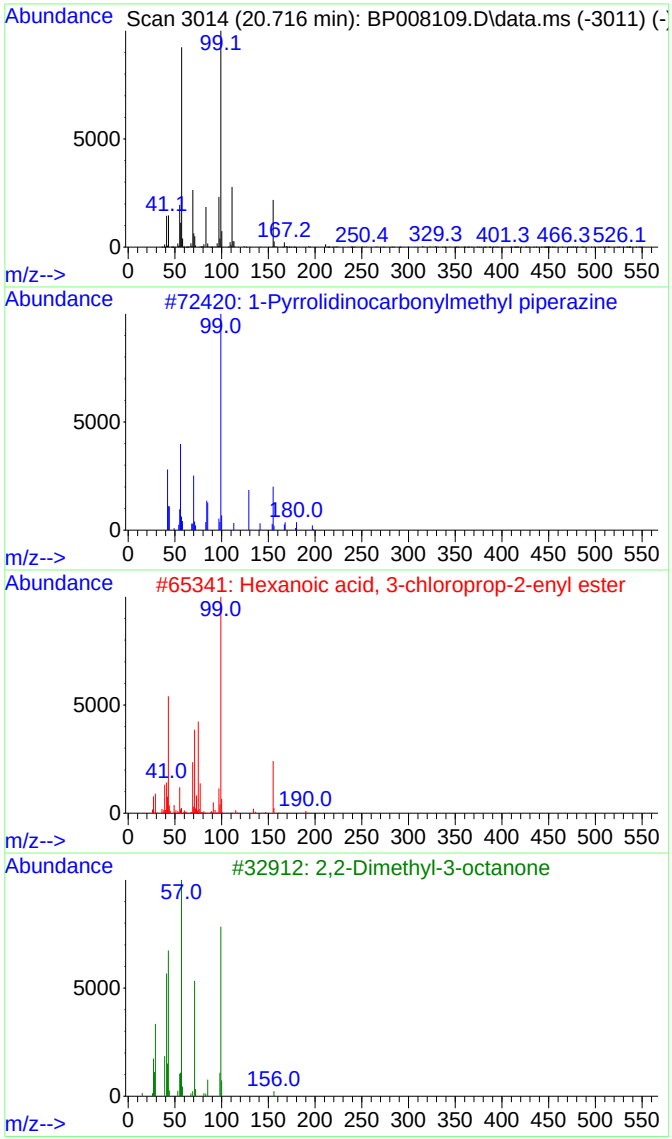
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

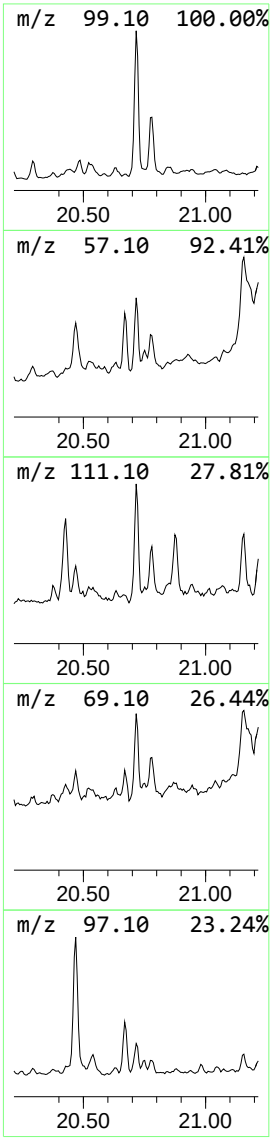
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 1-Pyrrolidinocarbonylmethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.716	9.45 ng	944854	Chrysene-d12	21.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pyrrolidinocarbonylmethyl pipe...	197	C10H19N3O	039890-45-4	50
2	Hexanoic acid, 3-chloroprop-2-en...	190	C9H15ClO2	1000299-36-1	47
3	2,2-Dimethyl-3-octanone	156	C10H20O	005340-64-7	38
4	Malonic acid, di(2,4-dimethylpen...	300	C17H32O4	1000349-02-5	38
5	N-Phenyl-N'-(2-piperazin-1-yl-et...	276	C14H20N4O2	332404-00-9	38





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Data File : BP008109.D
Acq On : 23 Nov 2021 22:25
Operator : CG/JU
Sample : M4803-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
266

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

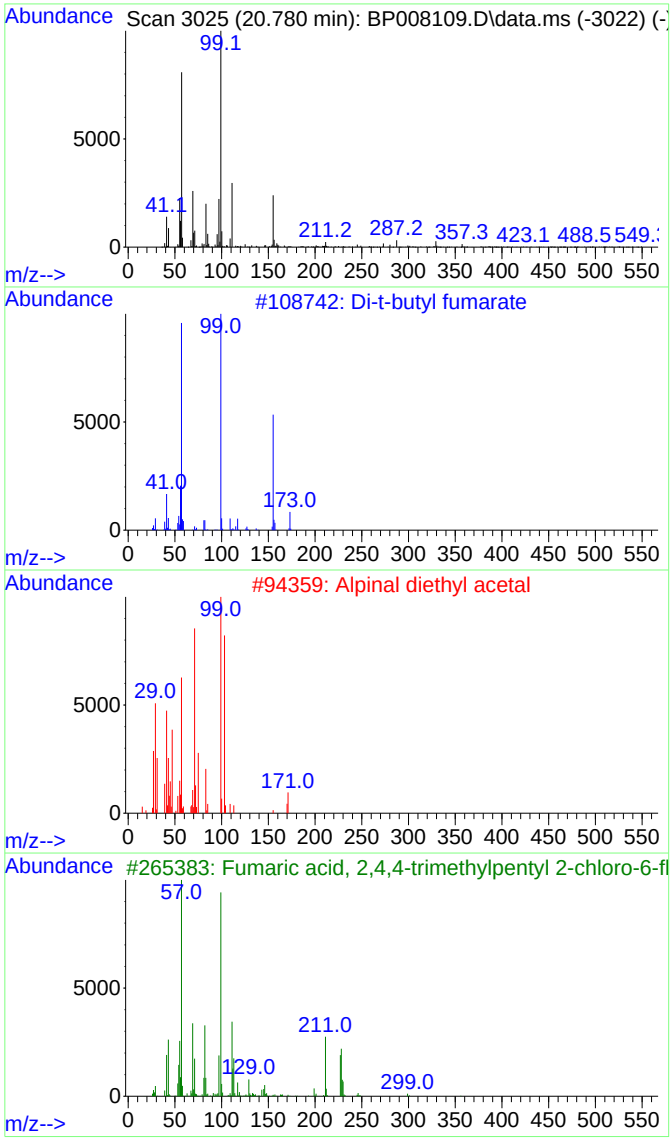
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

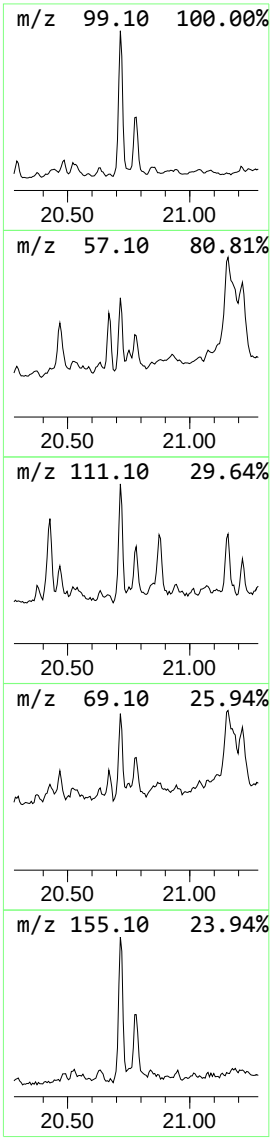
****

Peak Number 16 unknown20.780 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.780	6.97 ng	696785	Chrysene-d12	21.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-t-butyl fumarate	228	C12H20O4	007633-38-7	40
2	Alpinal diethyl acetal	216	C13H28O2	1000430-79-8	38
3	Fumaric acid, 2,4,4-trimethylpen...	356	C18H22ClFO4	1000405-60-9	36
4	4,8,12,16-Tetramethylheptadecan-...	324	C21H40O2	096168-15-9	32
5	trans-3-Methyl-4-octanolide	156	C9H16O2	039638-67-0	32





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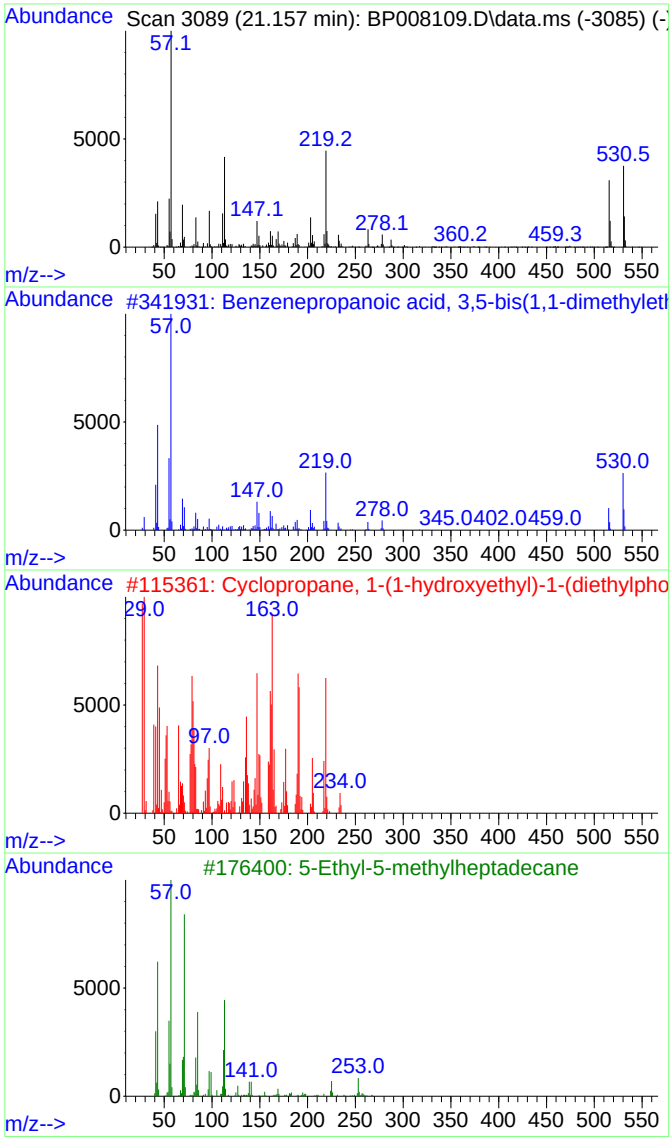
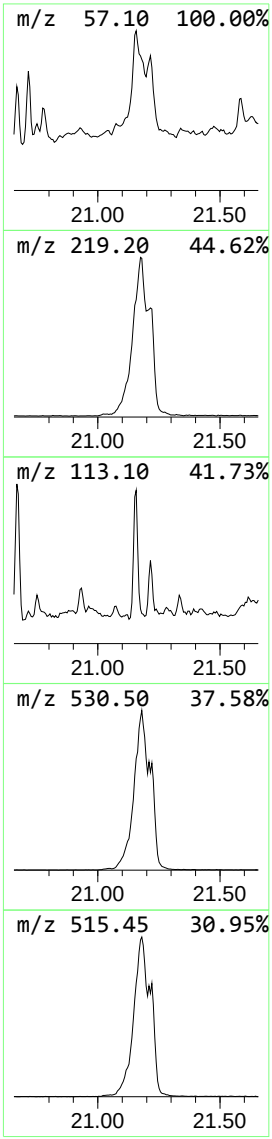
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 Benzenepropanoic acid, 3,5-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.157	15.97 ng	1596850	Chrysene-d12	21.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenepropanoic acid, 3,5-bis(1...	530	C35H62O3	002082-79-3	89
2	Cyclopropane, 1-(1-hydroxyethyl)...	234	C10H19O4P	1000157-94-9	15
3	5-Ethyl-5-methylheptadecane	282	C20H42	1000360-42-5	9
4	6,6-Dibutoxyhexanoic acid, butyl...	316	C18H36O4	1000280-29-0	9
5	5-Nonanone, 2,2,8,8-tetramethyl-	198	C13H26O	005709-95-5	9





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BNA_P
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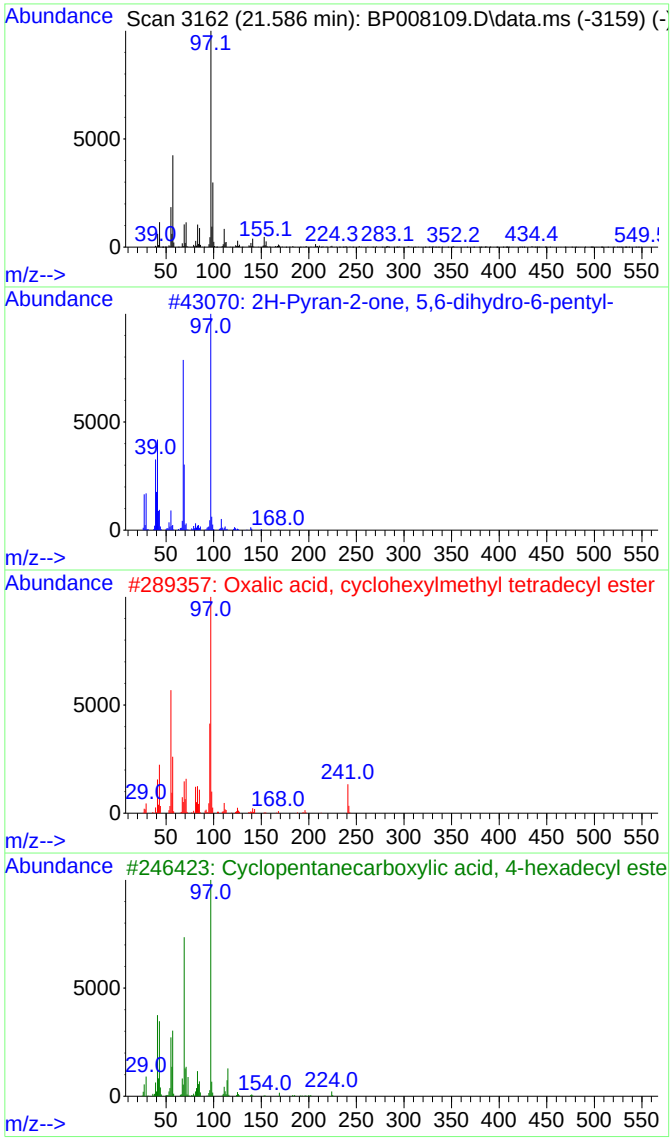
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

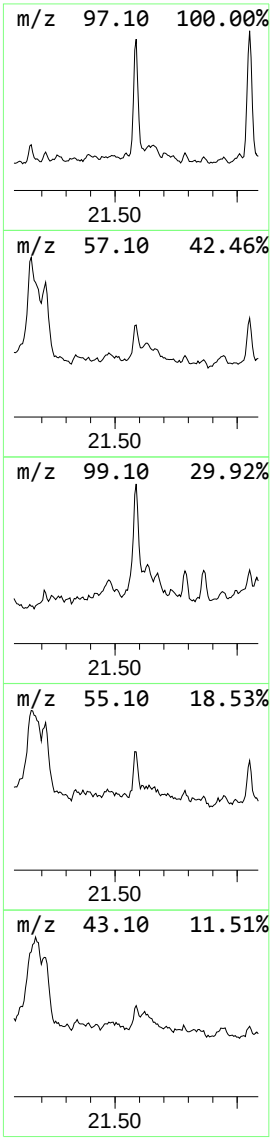
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 2H-Pyran-2-one, 5,6-dihydro... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.586	7.86 ng	785425	Chrysene-d12	21.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Pyran-2-one, 5,6-dihydro-6-pe...	168	C10H16O2	054814-64-1	50
2	Oxalic acid, cyclohexylmethyl te...	382	C23H42O4	1000309-69-0	50
3	Cyclopentanecarboxylic acid, 4-h...	338	C22H42O2	1000282-77-5	50
4	Oxalic acid, cyclohexylmethyl do...	354	C21H38O4	1000309-68-9	50
5	Oxalic acid, cyclohexylmethyl un...	340	C20H36O4	1000309-68-8	45





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

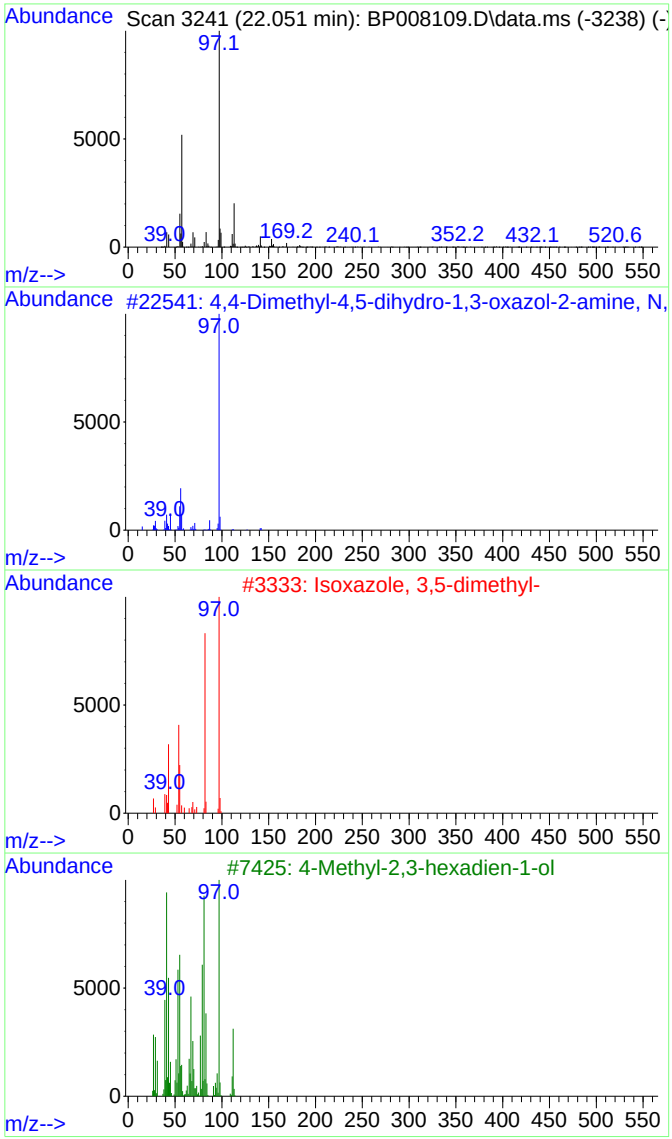
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

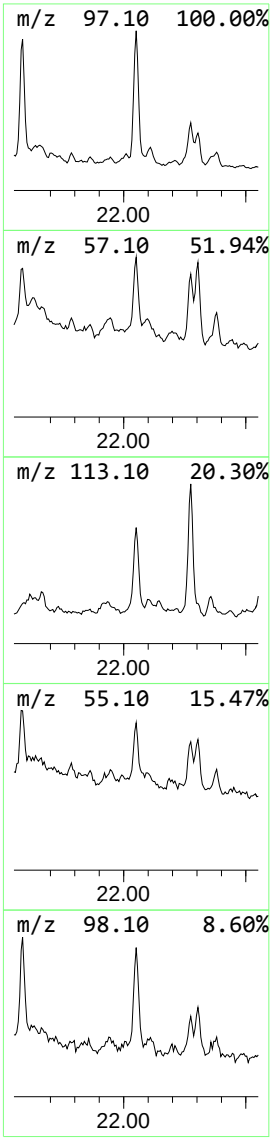
****

Peak Number 19 4,4-Dimethyl-4,5-dihydro-1,... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.051	7.03 ng	702775	Chrysene-d12	21.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4-Dimethyl-4,5-dihydro-1,3-oxa...	142	C7H14N2O	023802-98-4	50
2	Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	47
3	4-Methyl-2,3-hexadien-1-ol	112	C7H12O	1000196-09-6	47
4	2-[(2-Thienylmethyl)amino]-1-but...	185	C9H15NOS	156543-22-5	40
5	Bis(3,7-dimethyloctyl) methylpho...	376	C21H45O3P	1000298-35-2	40





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Sample : M4803-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

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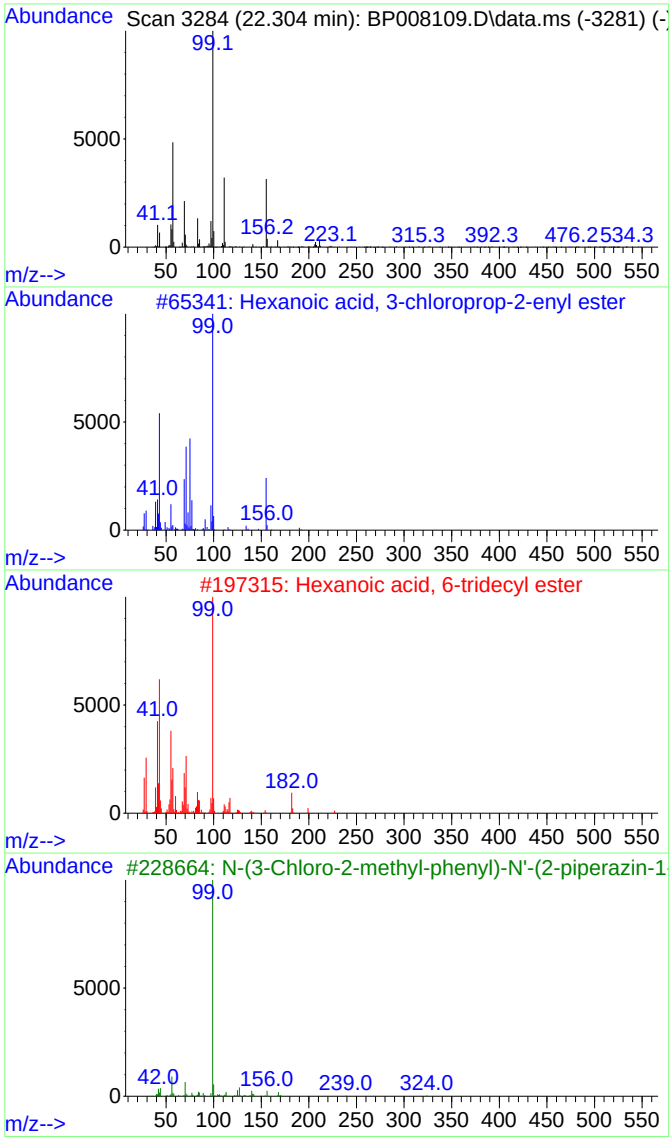
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

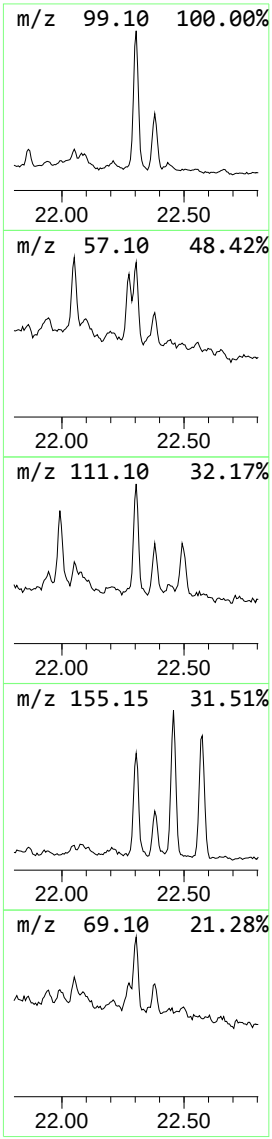
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 Hexanoic acid, 3-chloroprop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.304	9.67 ng	967207	Chrysene-d12	21.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3-chloroprop-2-en...	190	C9H15ClO2	1000299-36-1	64
2	Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	50
3	N-(3-Chloro-2-methyl-phenyl)-N'-...	324	C15H21ClN4O2	1000294-79-6	47
4	2,5-pyrrolidinedione, 3-dodecyl-	267	C16H29NO2	1000401-67-9	47
5	4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	45





Tentatively Identified Compound (LSC) summary

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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
Nonane	7.452	10.4	ng	476849	1	7.822	920496	20.0
Undecane	9.057	7.4	ng	338563	1	7.822	920496	20.0
Tetradecane	12.057	12.8	ng	1207040	2	10.622	1886410	20.0
2,4,4,6,6,8,8-H...	13.257	5.5	ng	517880	3	14.469	1873280	20.0
2-Azido-2,4,4,6...	13.528	7.3	ng	680725	3	14.469	1873280	20.0
unknown16.463	16.463	7.2	ng	821977	4	17.228	2281810	20.0
1-Methylnonyl m...	16.622	8.8	ng	998119	4	17.228	2281810	20.0
unknown17.310	17.310	6.8	ng	775502	4	17.228	2281810	20.0
Isoxazole, 3,5-...	18.022	10.7	ng	1222730	4	17.228	2281810	20.0
unknown18.945	18.945	9.3	ng	1063790	4	17.228	2281810	20.0
unknown19.480	19.480	5.7	ng	573075	5	21.322	1999480	20.0
unknown19.998	19.998	7.2	ng	718686	5	21.322	1999480	20.0
Succinic acid, ...	20.469	8.2	ng	824224	5	21.322	1999480	20.0
unknown20.669	20.669	5.8	ng	577010	5	21.322	1999480	20.0
1-Pyrrolidinoca...	20.716	9.4	ng	944854	5	21.322	1999480	20.0
unknown20.780	20.780	7.0	ng	696785	5	21.322	1999480	20.0
Benzenepropanoi...	21.157	16.0	ng	1596850	5	21.322	1999480	20.0
2H-Pyran-2-one,...	21.586	7.9	ng	785425	5	21.322	1999480	20.0
4,4-Dimethyl-4,...	22.051	7.0	ng	702775	5	21.322	1999480	20.0
Hexanoic acid, ...	22.304	9.7	ng	967207	5	21.322	1999480	20.0