LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028548.D
Acq On : 26 Jan 2021 19:33
Operator : CG/JU
Sample : M1217-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1525

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-BM012021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028548.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.434	37	42	51	rVB	8194	10316	1.04%	0.113%
2	5.034	308	314	322	rBV	22298	32809	3.30%	0.358%
3	5.516	390	396	406	rVB	334031	482390	48.57%	5.270%
4	6.034	478	484	494	rBV	20813	31010	3.12%	0.339%
5	7.146	667	673	686	rVB	299782	529870	53.36%	5.788%
6	7.522	732	737	742	rBV	45318	66674	6.71%	0.728%
7	7.581	742	747	756	rVB	50136	79968	8.05%	0.874%
8	7.769	773	779	790	rVB	69616	109033	10.98%	1.191%
9	7.993	809	817	823	rBV	125470	201000	20.24%	2.196%
10	9.163	1009	1016	1026	rBV	249367	401372	40.42%	4.385%
11	9.387	1048	1054	1059	rVB2	8440	13029	1.31%	0.142%
12	10.139	1172	1182	1191	rVB	34167	66651	6.71%	0.728%
13	10.316	1201	1212	1227	rBV5	9838	33884	3.41%	0.370%
14	10.575	1249	1256	1263	rBV2	5688	11157	1.12%	0.122%
15	10.745	1279	1285	1289	rBV5	5209	10978	1.11%	0.120%
16	10.804	1289	1295	1301	rVV	167735	272127	27.40%	2.973%
17	10.863	1301	1305	1315	rVB4	11455	21054	2.12%	0.230%
18	10.998	1323	1328	1335	rVB	7719	13137	1.32%	0.144%
19	11.163	1348	1356	1361	rBV3	7784	13162	1.33%	0.144%
20	11.586	1422	1428	1437	rBV3	5870	12122	1.22%	0.132%
21	13.257	1703	1712	1719	rVB	588486	853249	85.92%	9.321%
22	13.445	1740	1744	1747	rBV	10705	15705	1.58%	0.172%
23	13.951	1826	1830	1837	rVB7	5649	12992	1.31%	0.142%
24	14.039	1837	1845	1848	rBV5	5360	11286	1.14%	0.123%
25	14.080	1848	1852	1861	rVB	30646	49271	4.96%	0.538%
26	14.274	1879	1885	1894	rVB	30101	50845	5.12%	0.555%
27	14.574	1932	1936	1940	rBV	13974	21166	2.13%	0.231%
28	14.633	1940	1946	1954	rVB	243734	358961	36.15%	3.921%
29	14.774	1965	1970	1975	rBV8	7380	14533	1.46%	0.159%
30	14.822	1975	1978	1982	rVV3	9128	14532	1.46%	0.159%
31	14.880	1984	1988	1993	rVB	18269	26821	2.70%	0.293%
32	15.045	2011	2016	2024	rVB	73841	108732	10.95%	1.188%
33	15.133	2027	2031	2037	rBV6	8680	20340	2.05%	0.222%
34	15.263	2048	2053	2062	rVB2	27446	44992	4.53%	0.492%
35	15.410	2074	2078	2081	rBV	16319	22866	2.30%	0.250%
36	15.863	2149	2155	2160	rBV	21694	41457	4.17%	0.453%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028548.D
Acq On : 26 Jan 2021 19:33
Operator : CG/JU
Sample : M1217-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1525

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-BM012021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.933	2163	2167	2178	rVV2	43075	73939	7.45%	0.808%
38	16.116	2192	2198	2203	rBV	296959	421790	42.47%	4.608%
39	16.245	2218	2220	2224	rBV4	8755	15725	1.58%	0.172%
40	16.280	2224	2226	2229	rVB3	9939	10893	1.10%	0.119%
41	16.339	2230	2236	2240	rBV	56296	91124	9.18%	0.995%
42	16.586	2275	2278	2282	rVB2	15014	19717	1.99%	0.215%
43	17.157	2371	2375	2379	rVB	46137	60068	6.05%	0.656%
44	17.263	2391	2393	2397	rVB3	16331	17067	1.72%	0.186%
45	17.363	2404	2410	2415	rBV	274571	388999	39.17%	4.250%
46	17.568	2443	2445	2452	rVB2	14847	18252	1.84%	0.199%
47	18.239	2554	2559	2568	rBV	301652	404604	40.74%	4.420%
48	18.733	2639	2643	2647	rVB2	33688	52484	5.28%	0.573%
49	18.992	2682	2687	2691	rVB	244226	305935	30.81%	3.342%
50	19.074	2698	2701	2709	rVB	80456	109231	11.00%	1.193%
51	19.145	2710	2713	2720	rVB2	27225	43493	4.38%	0.475%
52	19.504	2769	2774	2782	rBV	124265	180023	18.13%	1.967%
53	19.615	2790	2793	2801	rVB	65381	80186	8.07%	0.876%
54	19.680	2802	2804	2808	rBV	17066	20208	2.03%	0.221%
55	19.956	2846	2851	2858	rVB	794747	993087	100.00%	10.849%
56	20.145	2880	2883	2889	rVB	35314	44721	4.50%	0.489%
57	20.621	2960	2964	2969	rVB	56562	74460	7.50%	0.813%
58	20.739	2981	2984	2988	rVB	26287	31238	3.15%	0.341%
59	20.827	2995	2999	3003	rBV	159772	182907	18.42%	1.998%
60	20.868	3003	3006	3010	rVB	33540	36603	3.69%	0.400%
61	21.198	3057	3062	3072	rBV	352207	438839	44.19%	4.794%
62	21.492	3108	3112	3118	rVB	275081	356220	35.87%	3.891%
63	21.627	3132	3135	3141	rBV2	31310	38232	3.85%	0.418%
64	22.062	3206	3209	3212	rBV	27247	40443	4.07%	0.442%
65	22.527	3286	3288	3293	rVB	24232	28547	2.87%	0.312%
66	23.762	3492	3498	3506	rVB2	182062	349418	35.19%	3.817%
67	24.374	3597	3602	3612	rVB	63198	145980	14.70%	1.595%

Sum of corrected areas: 9153924

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
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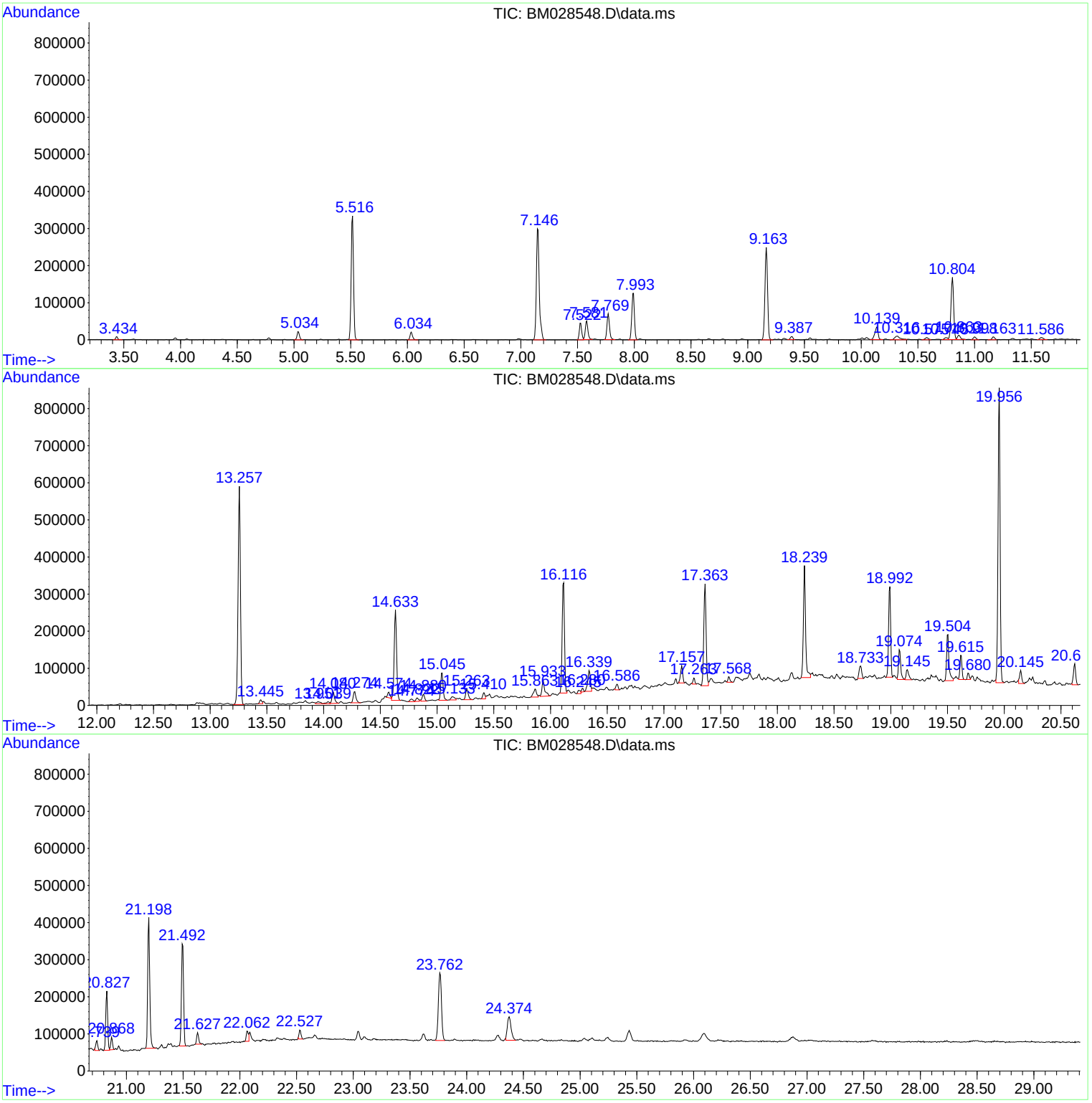
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
1525

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028548.D
Acq On : 26 Jan 2021 19:33
Operator : CG/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

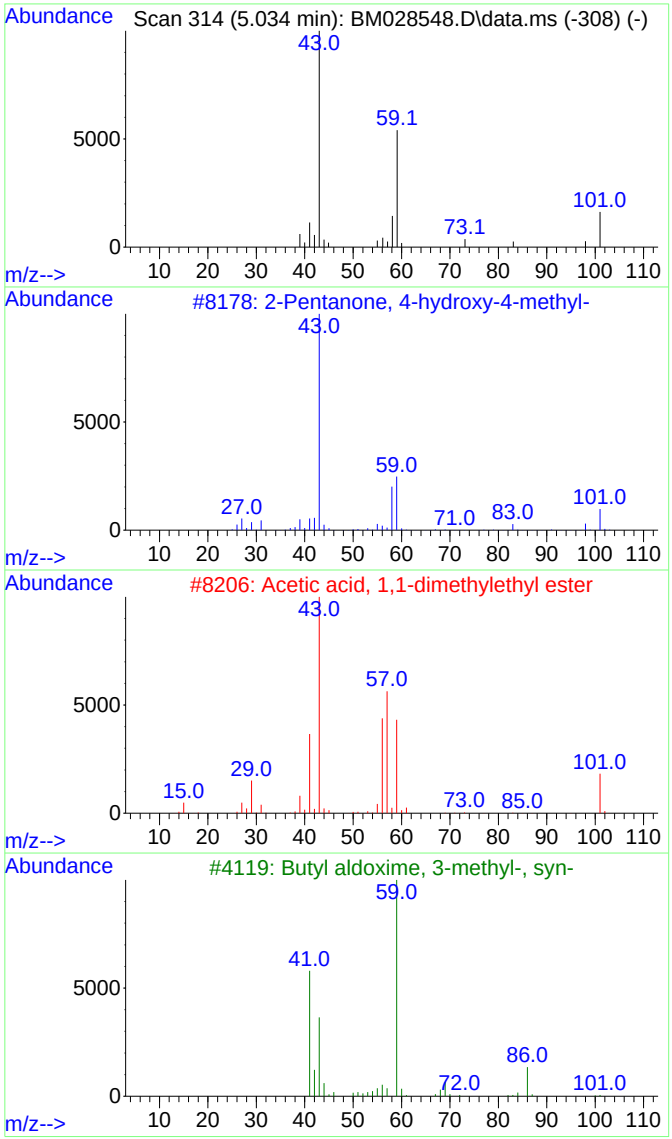
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

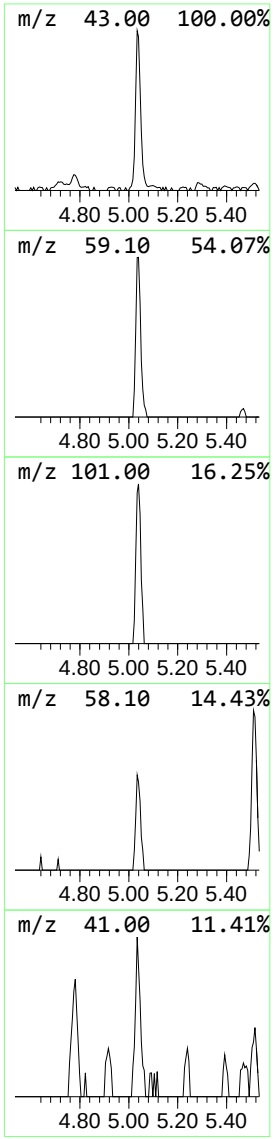
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	3.26 ng	32809	1,4-Dichlorobenzene-d4	7.993

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028548.D
Acq On : 26 Jan 2021 19:33
Operator : CG/JU
Sample : M1217-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1525

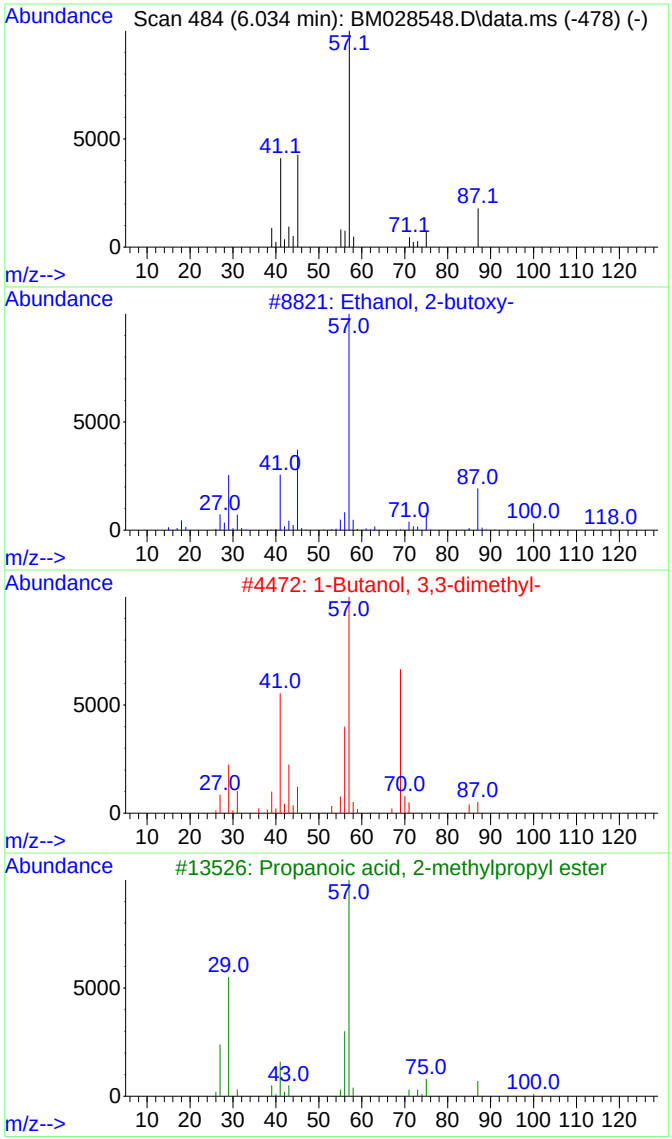
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

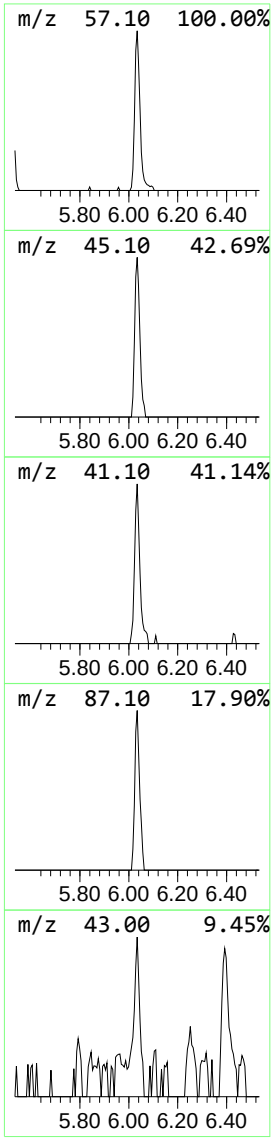
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-butoxy- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.034	3.09 ng	31010	1,4-Dichlorobenzene-d4	7.993

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
2	1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	23
3	Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	17
4	1-Butene, 4-butoxy-	128	C8H16O	034061-76-2	12
5	Propanedioic acid, oxo-, bis(2-m...	230	C11H18O5	092778-43-3	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028548.D
Acq On : 26 Jan 2021 19:33
Operator : CG/JU
Sample : M1217-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1525

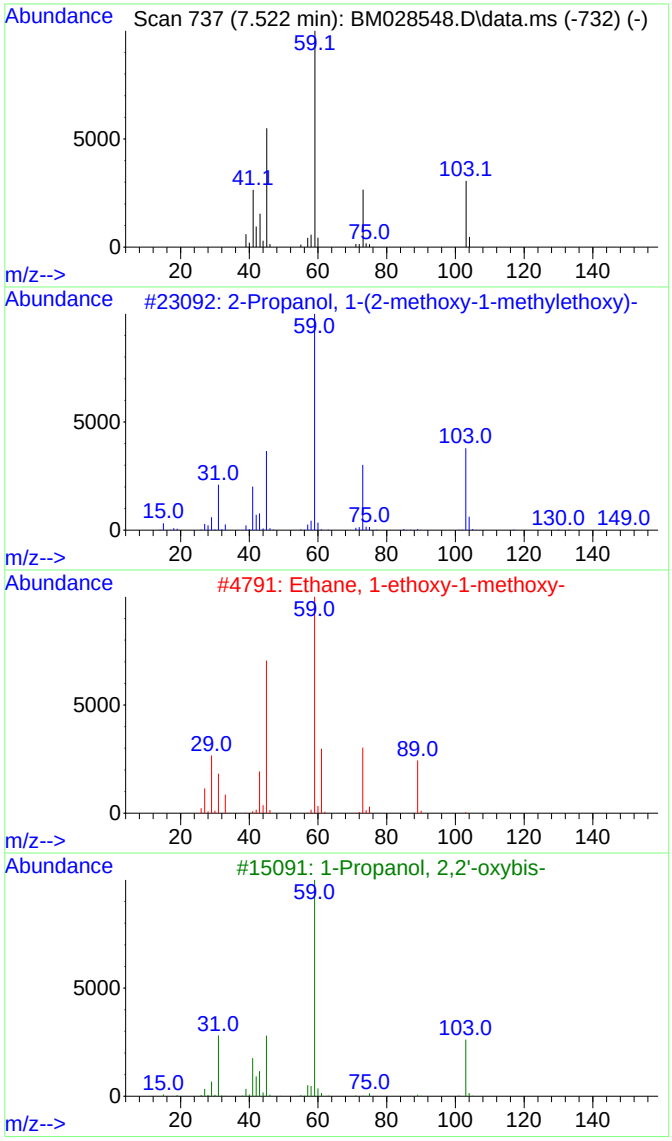
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

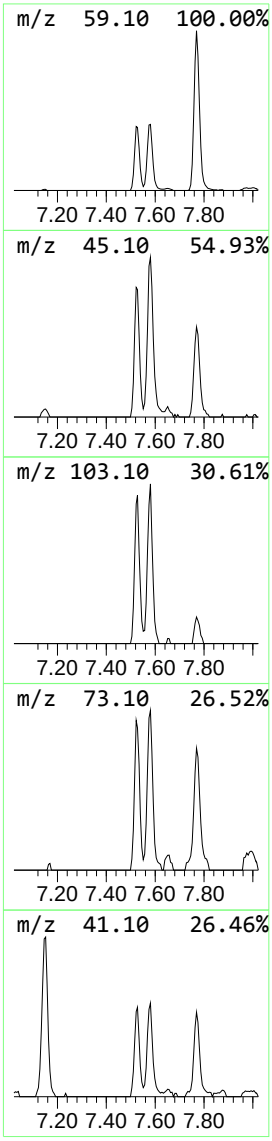
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.522	6.63 ng	66674	1,4-Dichlorobenzene-d4	7.993

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	86
2	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	59
3	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	59
4	1-Propanol, 3,3'-oxybis-	134	C6H14O3	002396-61-4	45
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028548.D
Acq On : 26 Jan 2021 19:33
Operator : CG/JU
Sample : M1217-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1525

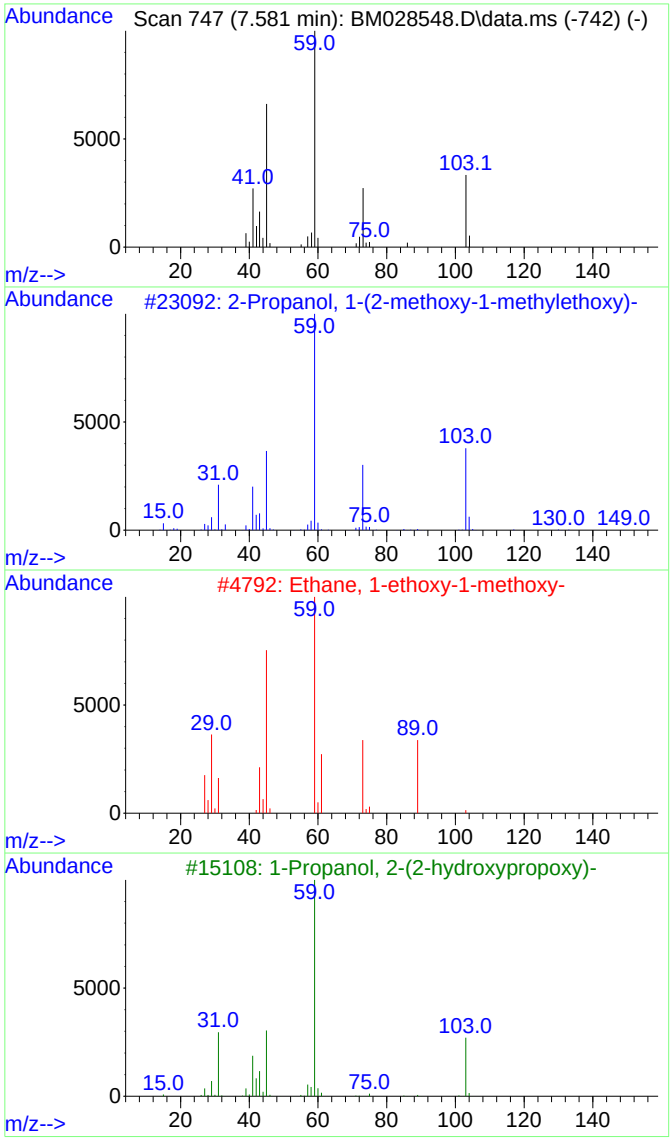
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

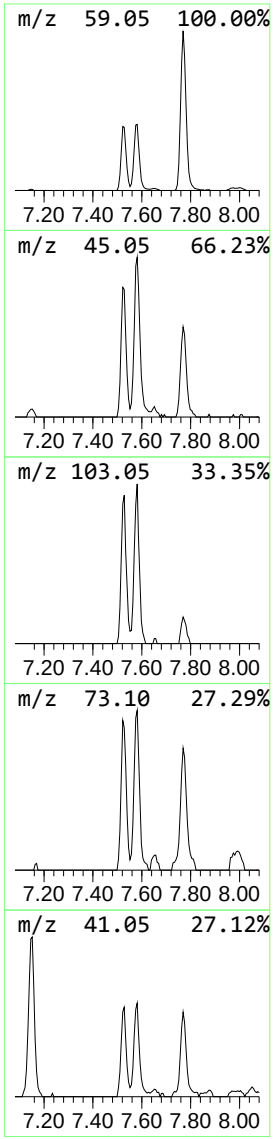
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethane, 1-ethoxy-1-methoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.581	7.96 ng	79968	1,4-Dichlorobenzene-d4	7.993

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72
2	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	59
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	53
5	2-Propanol, 1-(2-ethoxypropoxy)-	162	C8H18O3	010143-32-5	39





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028548.D
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Sample : M1217-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1525

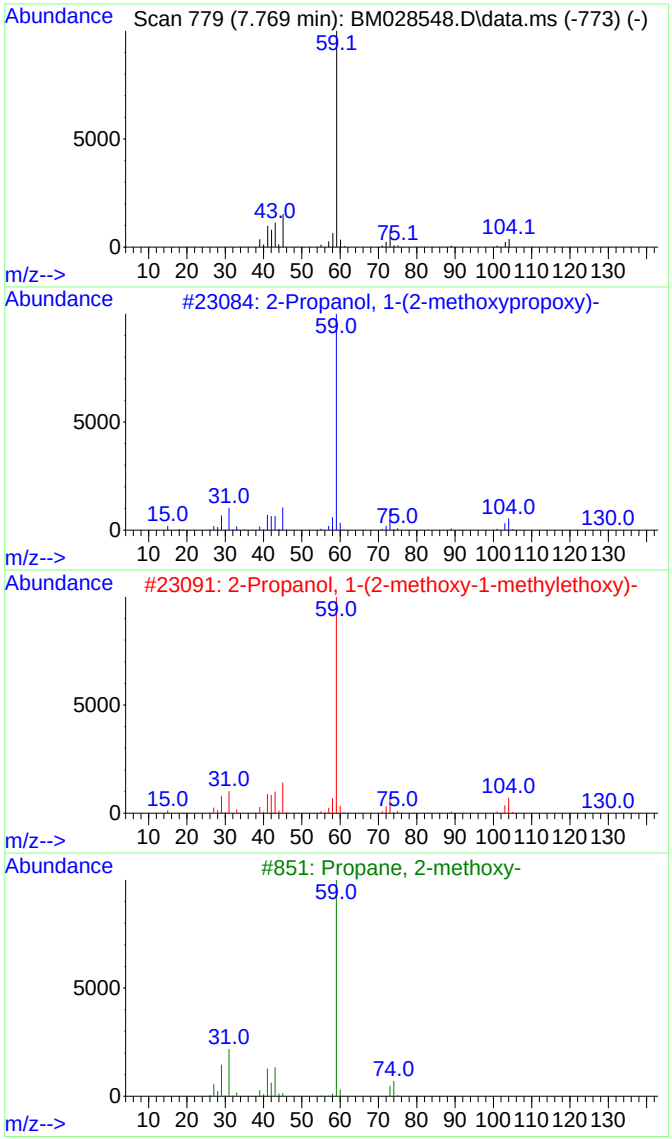
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

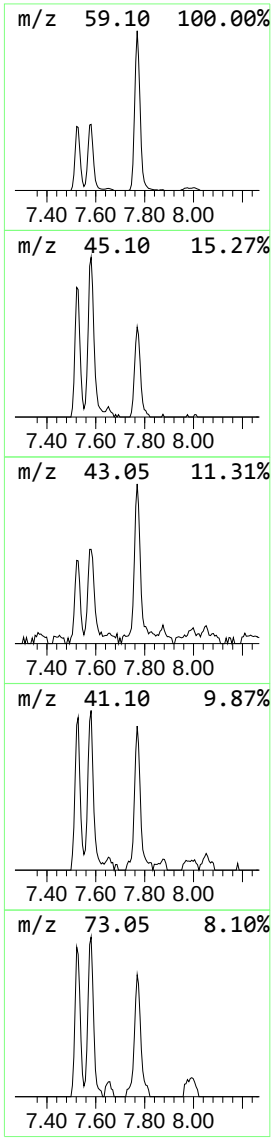
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Propanol, 1-(2-methoxypro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.769	10.85 ng	109033	1,4-Dichlorobenzene-d4	7.993

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	83
2	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	74
3	Propane, 2-methoxy-	74	C4H10O	000598-53-8	50
4	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	43
5	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	39





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

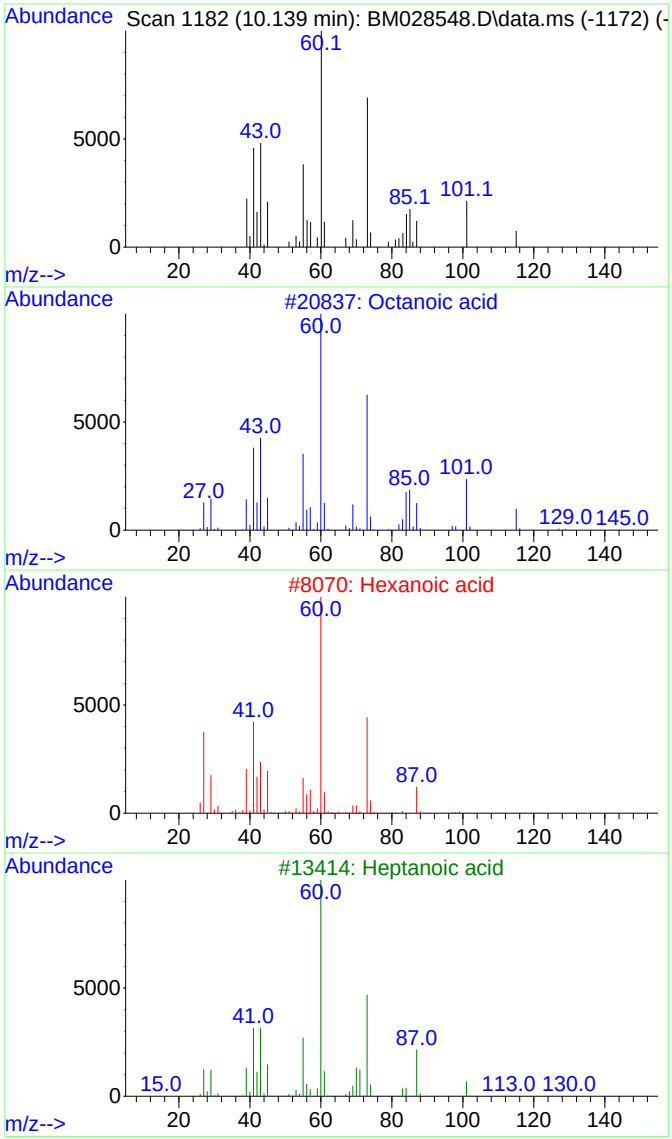
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

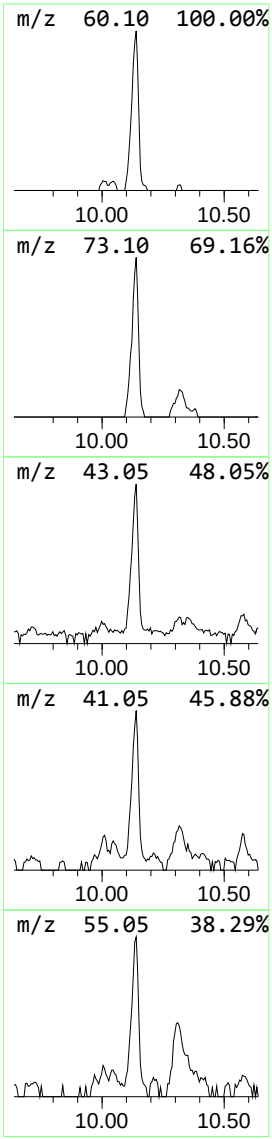
****

Peak Number 6 Octanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.140	4.90 ng	66651	Naphthalene-d8	10.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	90
2	Hexanoic acid	116	C6H12O2	000142-62-1	59
3	Heptanoic acid	130	C7H14O2	000111-14-8	50
4	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	42
5	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028548.D
Acq On : 26 Jan 2021 19:33
Operator : CG/JU
Sample : M1217-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1525

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

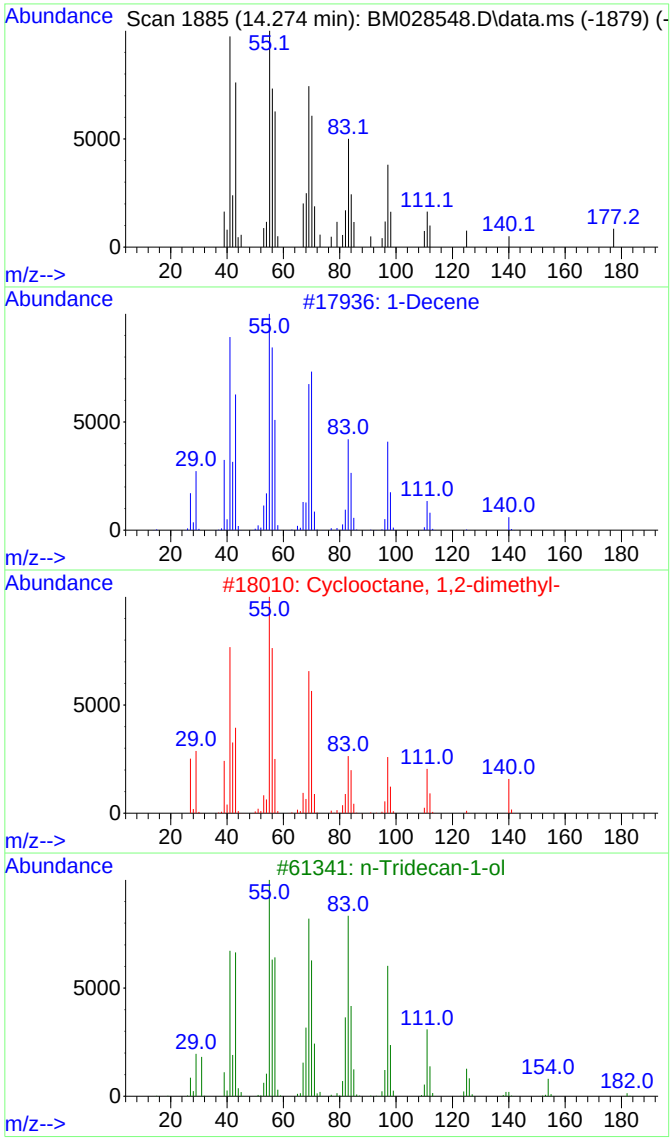
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

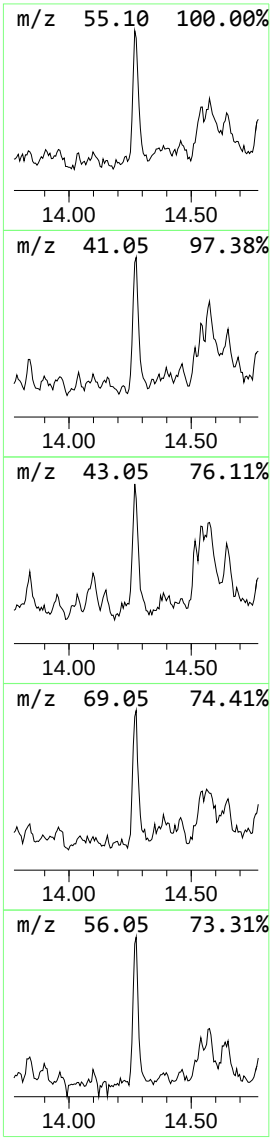
****

Peak Number 7 1-Decene Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.275	2.83 ng	50845	Acenaphthene-d10	14.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decene	140	C10H20	000872-05-9	96
2	Cyclooctane, 1,2-dimethyl-	140	C10H20	013151-94-5	90
3	n-Tridecan-1-ol	200	C13H28O	000112-70-9	90
4	Cyclododecane	168	C12H24	000294-62-2	90
5	Cyclopropane, nonyl-	168	C12H24	074663-85-7	86





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Data File : BM028548.D
Acq On : 26 Jan 2021 19:33
Operator : CG/JU
Sample : M1217-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1525

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

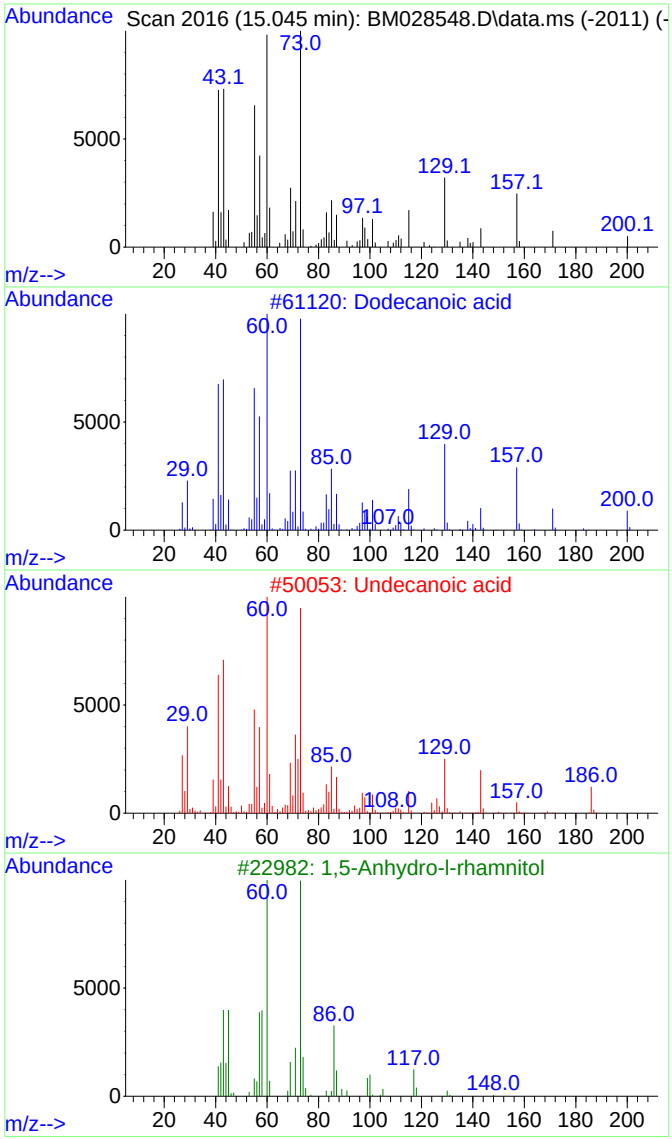
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

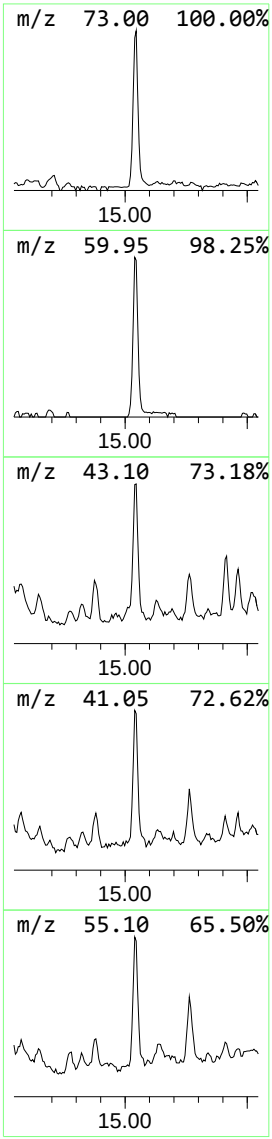
****

Peak Number 8 Dodecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.045	6.06 ng	108732	Acenaphthene-d10	14.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	98
2	Undecanoic acid	186	C11H22O2	000112-37-8	64
3	1,5-Anhydro-l-rhamnitol	148	C6H12O4	1000129-02-4	47
4	Octanoic acid	144	C8H16O2	000124-07-2	47
5	1,2,3,4-Cyclopentanetetrol, (1.a...	134	C5H10O4	014003-71-5	47





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Sample : M1217-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1525

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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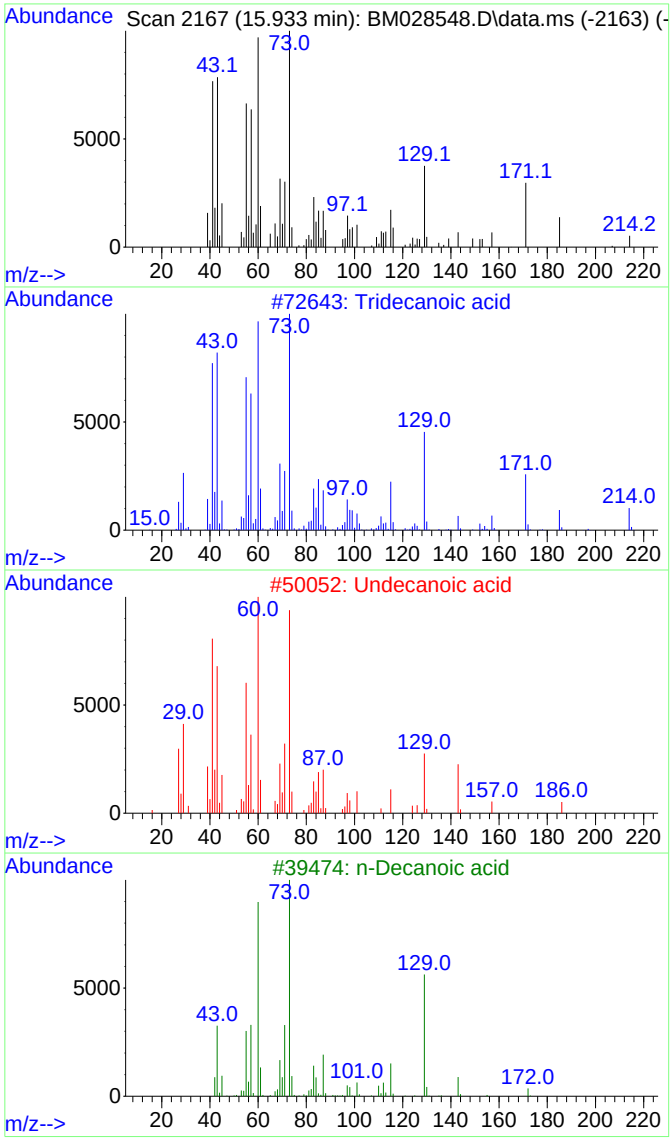
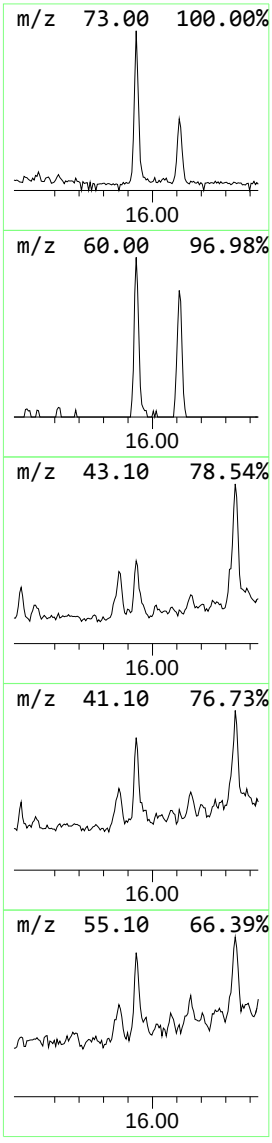
Peak Number 9 Tridecanoic acid Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.933	4.12 ng	73939	Acenaphthene-d10	14.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	80
2	Undecanoic acid	186	C11H22O2	000112-37-8	62
3	n-Decanoic acid	172	C10H20O2	000334-48-5	53
4	d-Glucohexodialdose	178	C6H10O6	1000149-19-1	43
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	43





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Operator : CG/JU
Sample : M1217-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1525

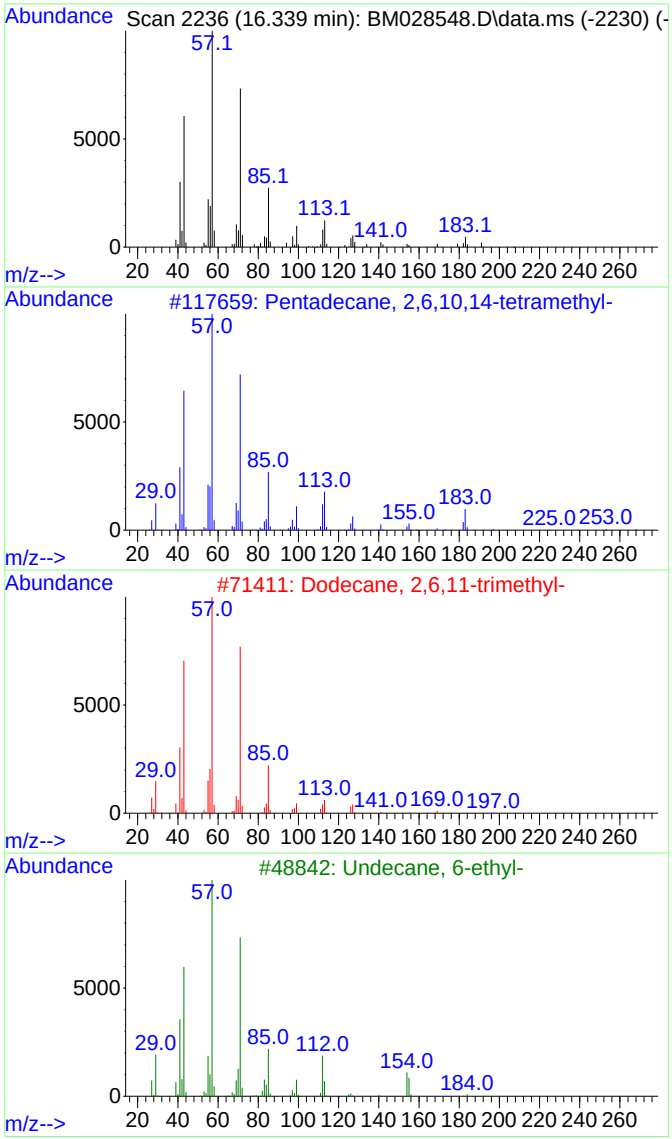
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

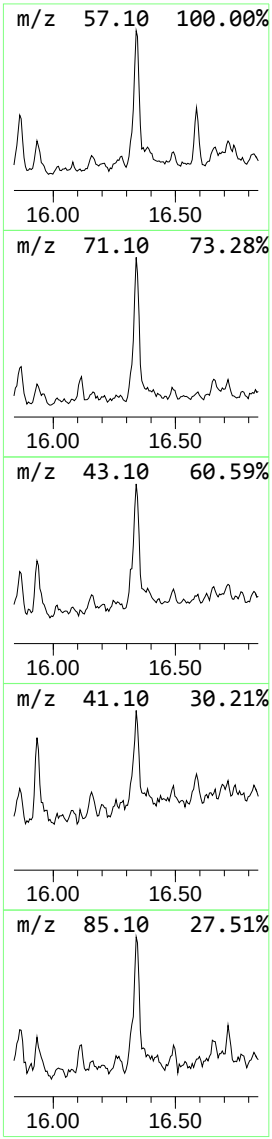
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Pentadecane, 2,6,10,14-tetr... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.339	4.69 ng	91124	Phenanthrene-d10	17.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	90
2	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	86
3	Undecane, 6-ethyl-	184	C13H28	017312-60-6	80
4	Tridecane, 5-propyl-	226	C16H34	055045-11-9	80
5	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	64





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Acq On : 26 Jan 2021 19:33
Operator : CG/JU
Sample : M1217-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1525

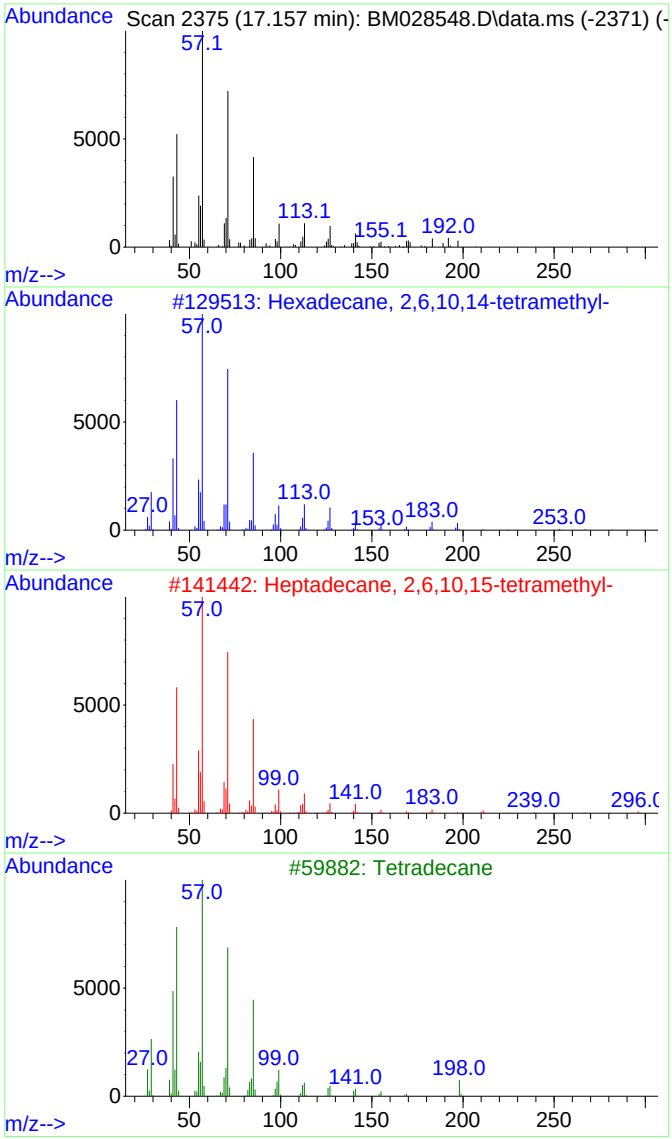
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

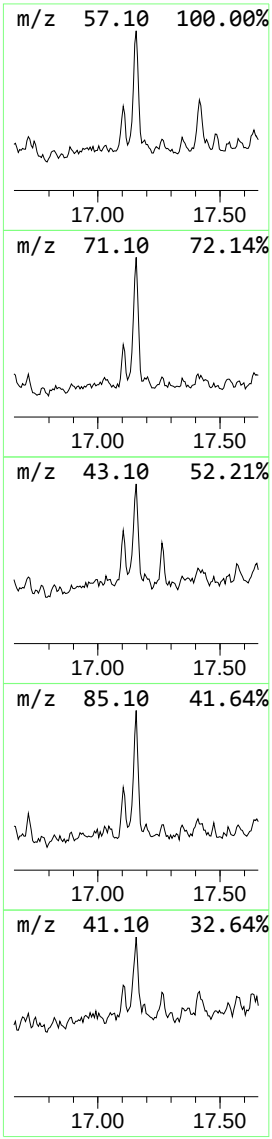
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Hexadecane, 2,6,10,14-tetra... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.157	3.09 ng	60068	Phenanthrene-d10	17.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	91
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
3	Tetradecane	198	C14H30	000629-59-4	86
4	Dodecane	170	C12H26	000112-40-3	83
5	5,5-Dibutylnonane	240	C17H36	006008-17-9	78





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Operator : CG/JU
Sample : M1217-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1525

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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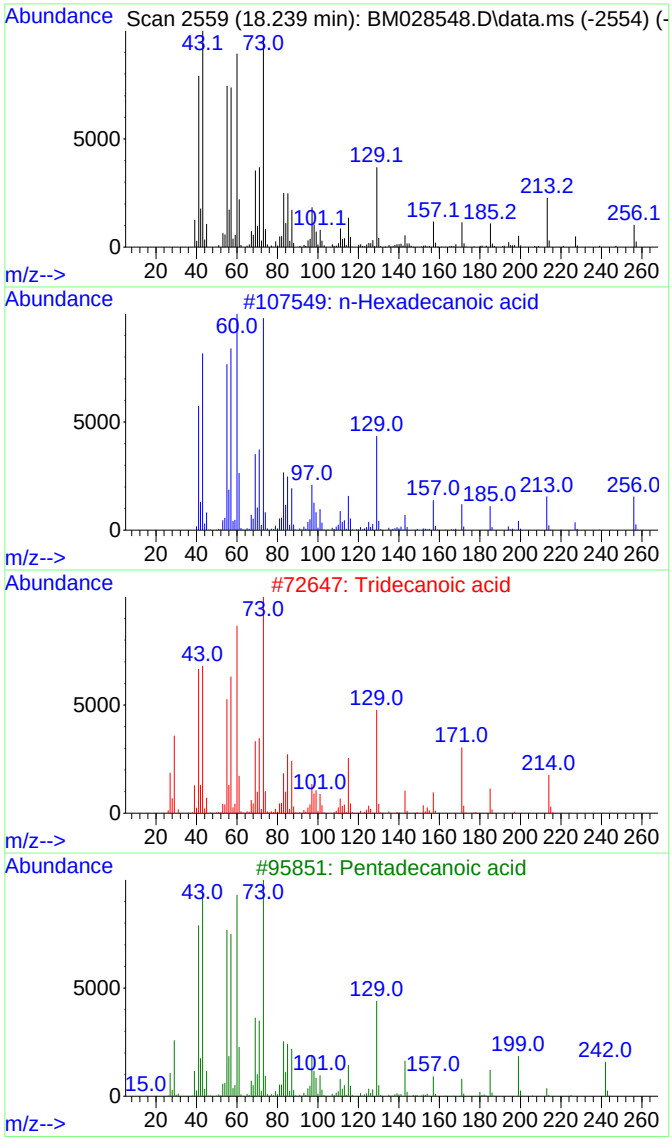
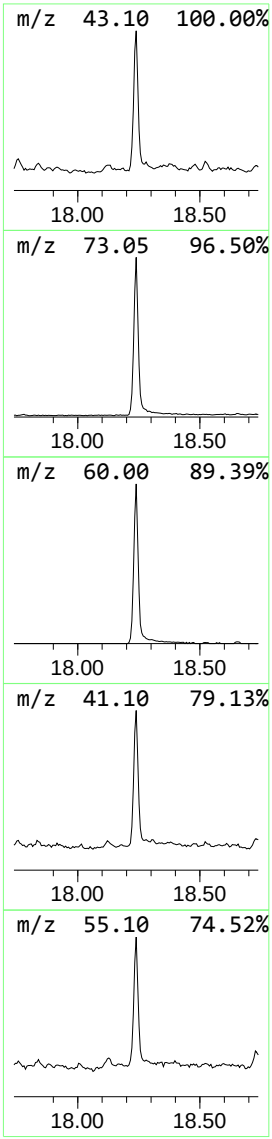
Peak Number 12 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.239	20.80 ng	404604	Phenanthrene-d10	17.363

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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Acq On : 26 Jan 2021 19:33
Operator : CG/JU
Sample : M1217-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1525

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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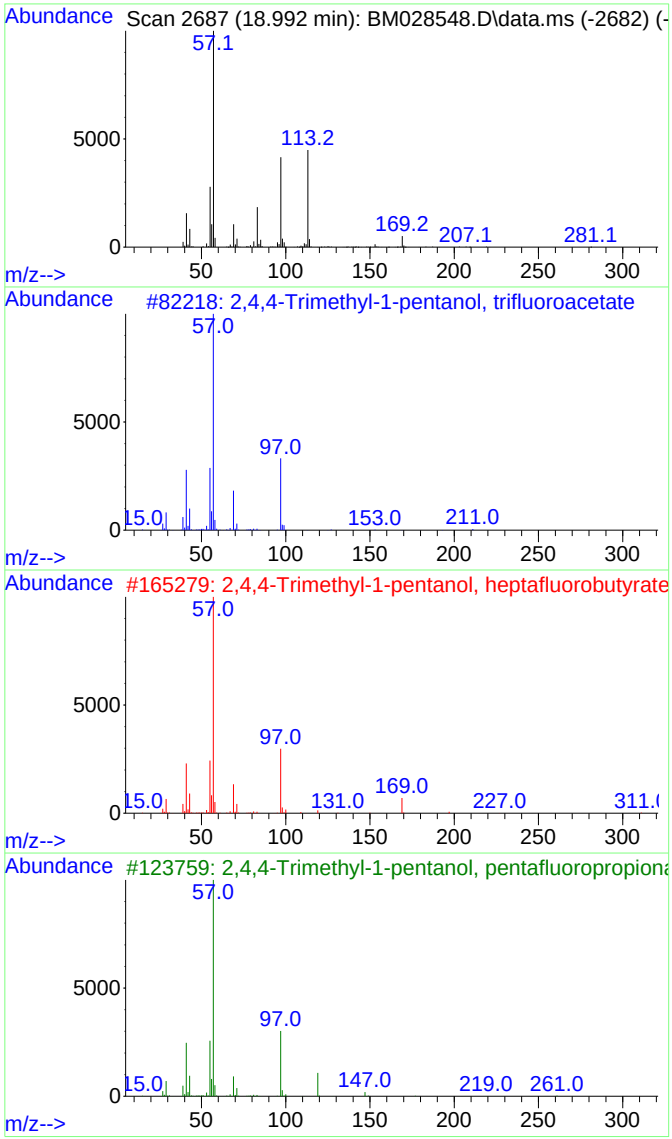
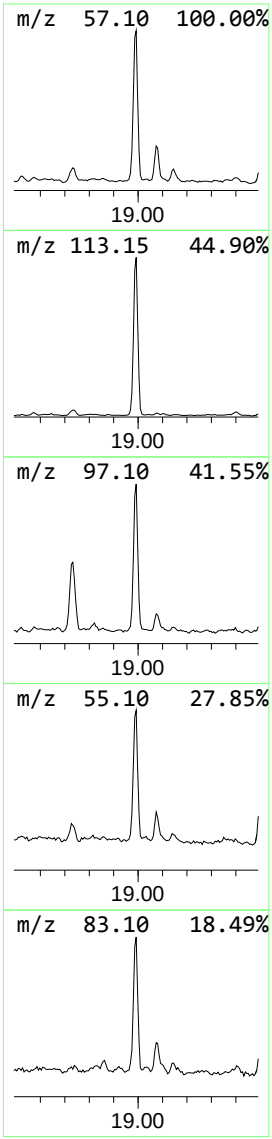
Peak Number 13 unknown18.992 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.992	15.73 ng	305935	Phenanthrene-d10	17.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	38
2	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	38
3	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	32
4	Octane, 2-iodo-	240	C8H17I	000557-36-8	28
5	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	28





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Operator : CG/JU
Sample : M1217-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1525

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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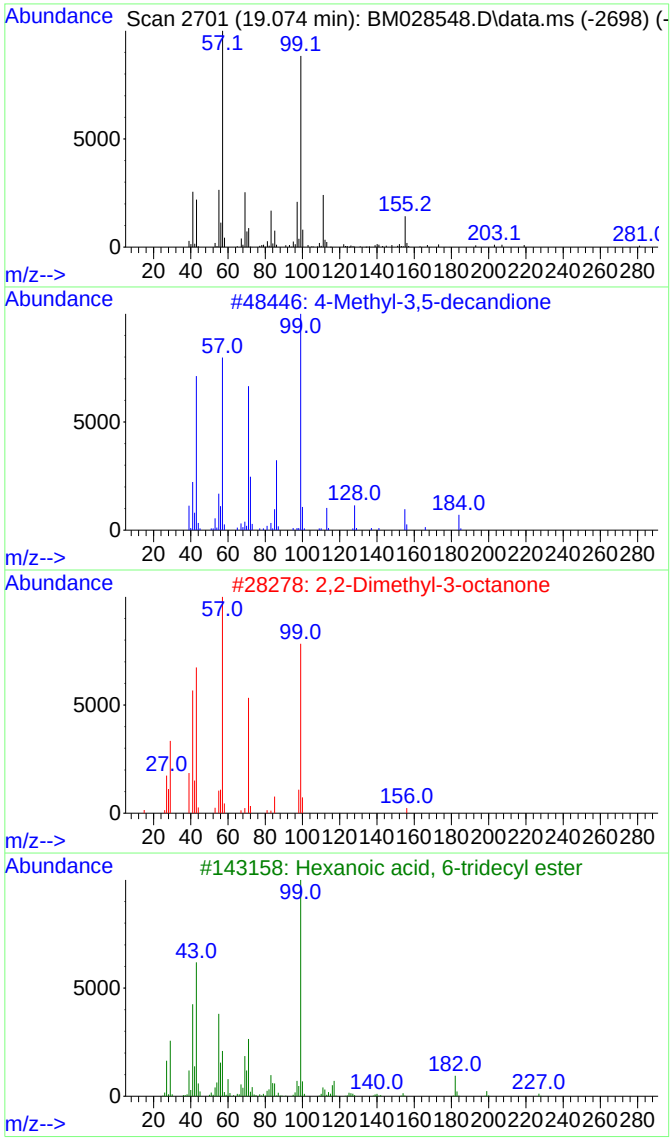
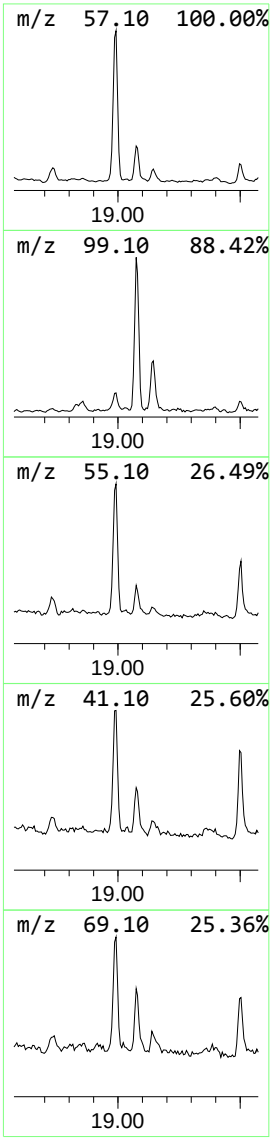
Peak Number 14 4-Methyl-3,5-decandione Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.074	5.62 ng	109231	Phenanthrene-d10	17.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyl-3,5-decandione	184	C11H20O2	1000374-13-1	50
2	2,2-Dimethyl-3-octanone	156	C10H20O	005340-64-7	50
3	Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	47
4	Hexanoic acid, 5-tridecyl ester	298	C19H38O2	1000279-29-4	40
5	(.+/-.)-Dethiobiotin	214	C10H18N2O3	000636-20-4	38





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Sample : M1217-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1525

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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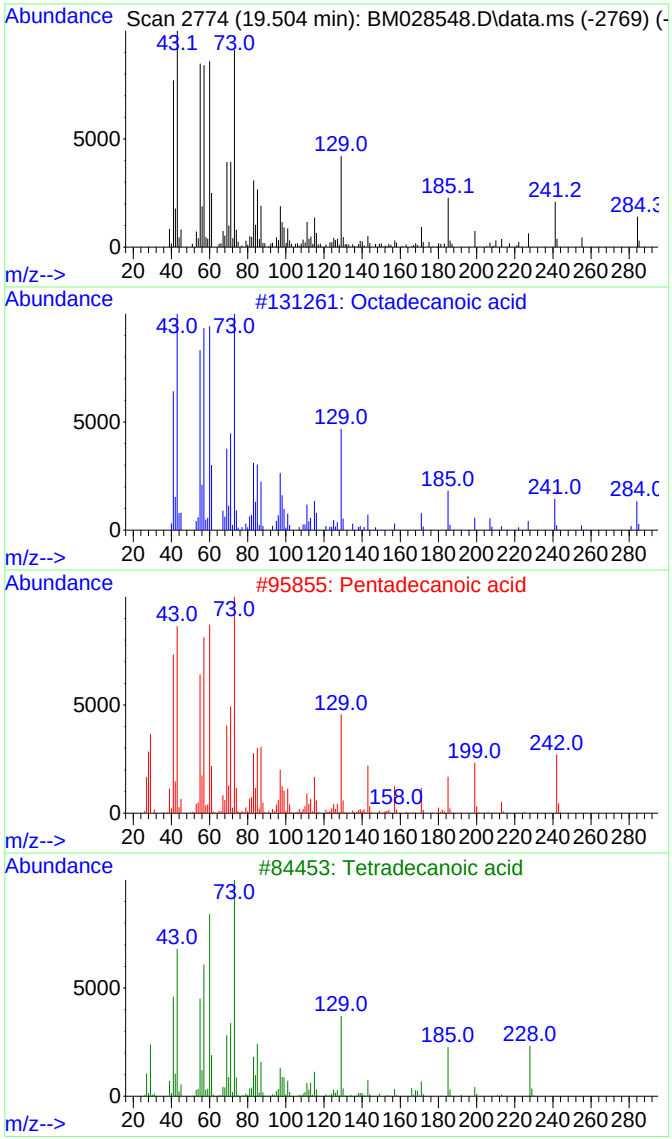
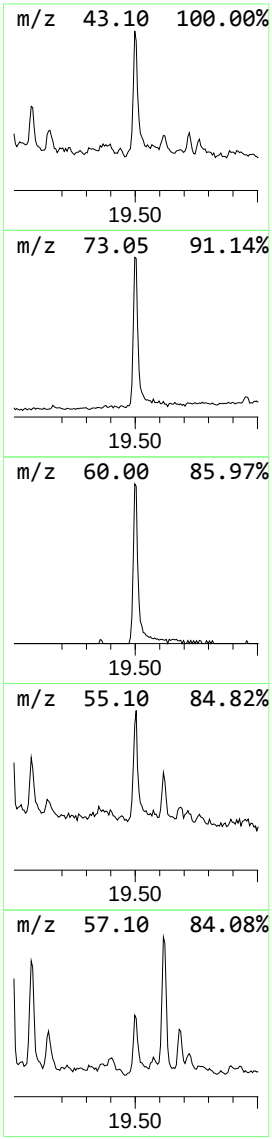
Peak Number 15 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.504	10.11 ng	180023	Chrysene-d12	21.492

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	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Sample : M1217-15
Misc :
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Instrument : BNA_M
ClientSampleId : 1525

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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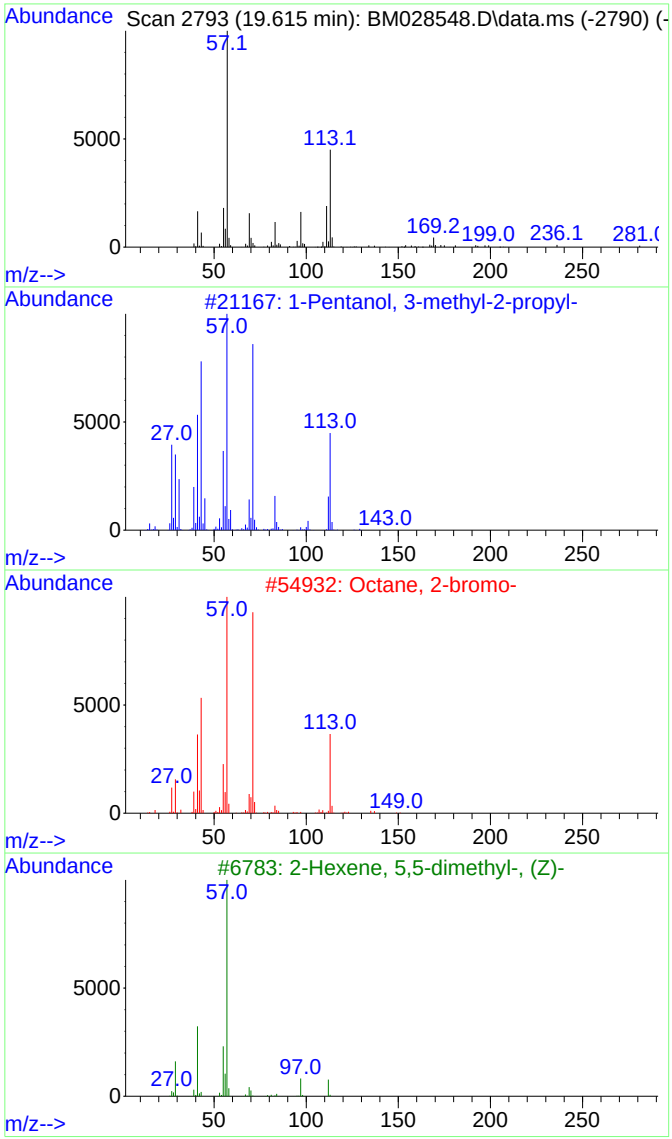
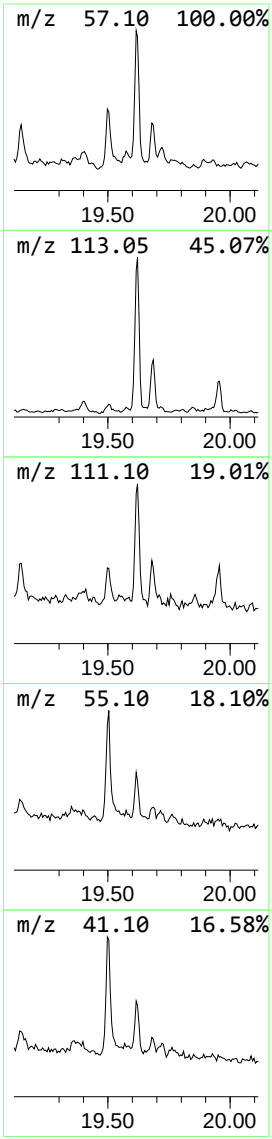
Peak Number 16 unknown19.615 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.615	4.50 ng	80186	Chrysene-d12	21.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	36
2	Octane, 2-bromo-	192	C8H17Br	000557-35-7	25
3	2-Hexene, 5,5-dimethyl-, (Z)-	112	C8H16	039761-61-0	14
4	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	14
5	Thiocyanic acid, 1,1,3,3-tetrame...	171	C9H17NS	089601-36-5	12





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1525

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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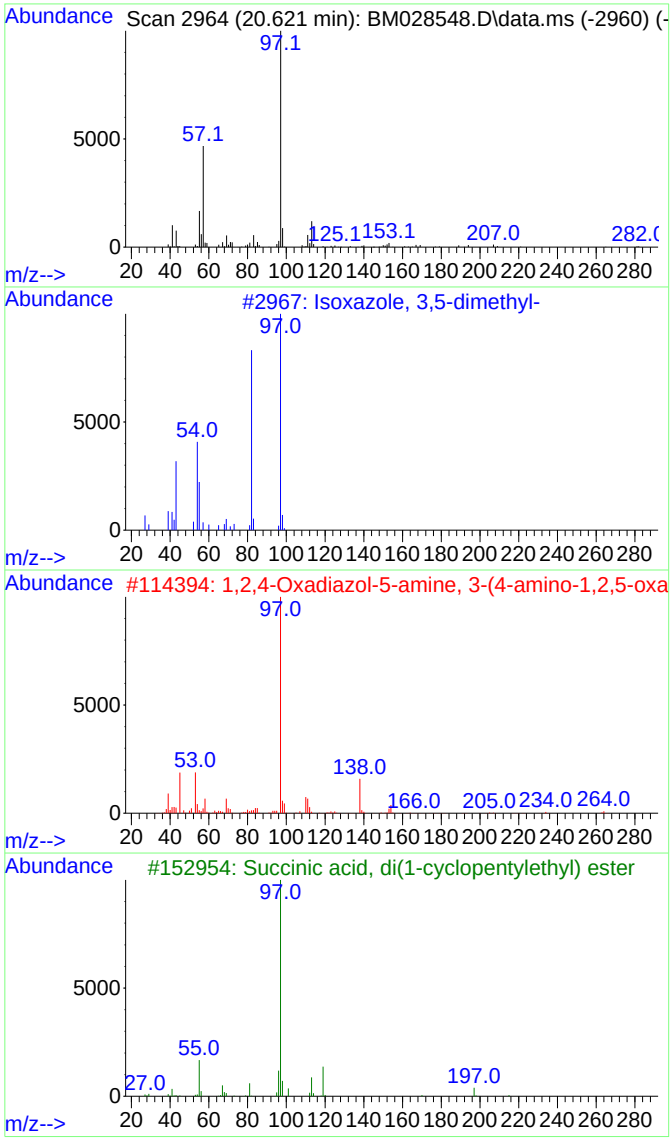
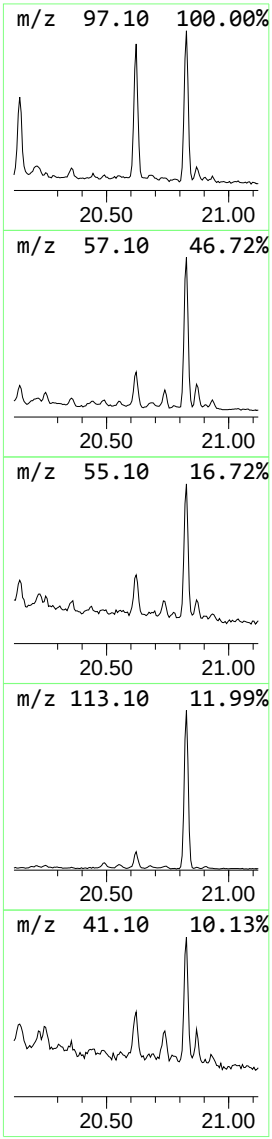
Peak Number 17 Isoxazole, 3,5-dimethyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.621	4.18 ng	74460	Chrysene-d12	21.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	58
2	1,2,4-Oxadiazol-5-amine, 3-(4-am...	264	C9H8N6O2S	1000351-26-9	53
3	Succinic acid, di(1-cyclopentyle...	310	C18H30O4	1000330-21-8	50
4	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	45
5	Thiophene, 3-ethyl-	112	C6H8S	001795-01-3	45





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Instrument : BNA_M
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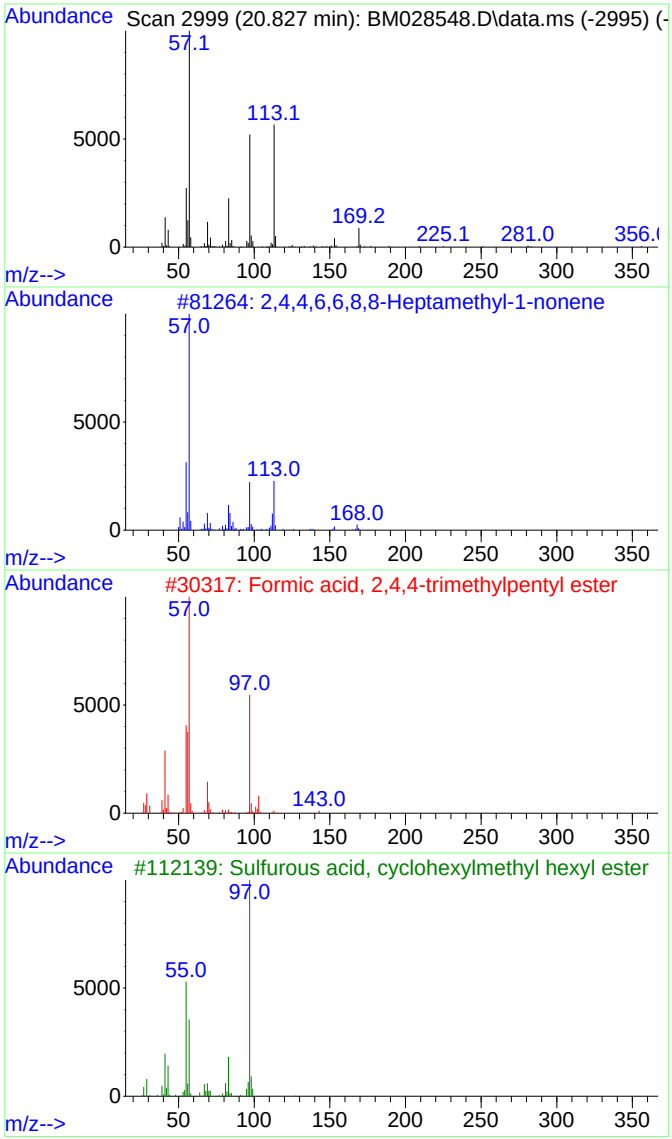
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

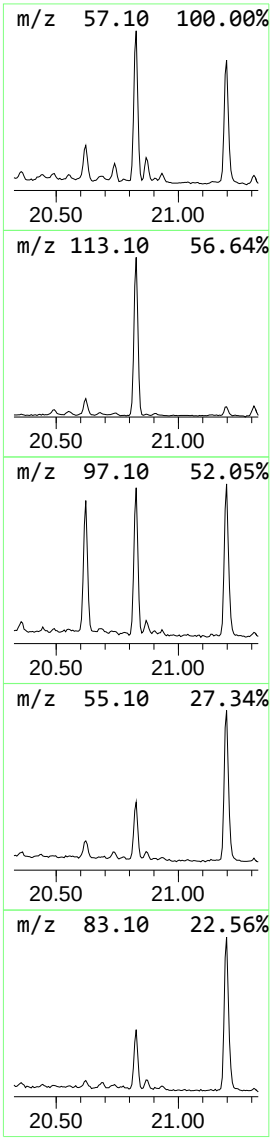
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.827	10.27 ng	182907	Chrysene-d12	21.492

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	74
2	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	32
3	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-6	32
4	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	27
5	Cyclopentanecarboxylic acid, 4-h...	338	C22H42O2	1000282-77-5	27





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Operator : CG/JU
Sample : M1217-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1525

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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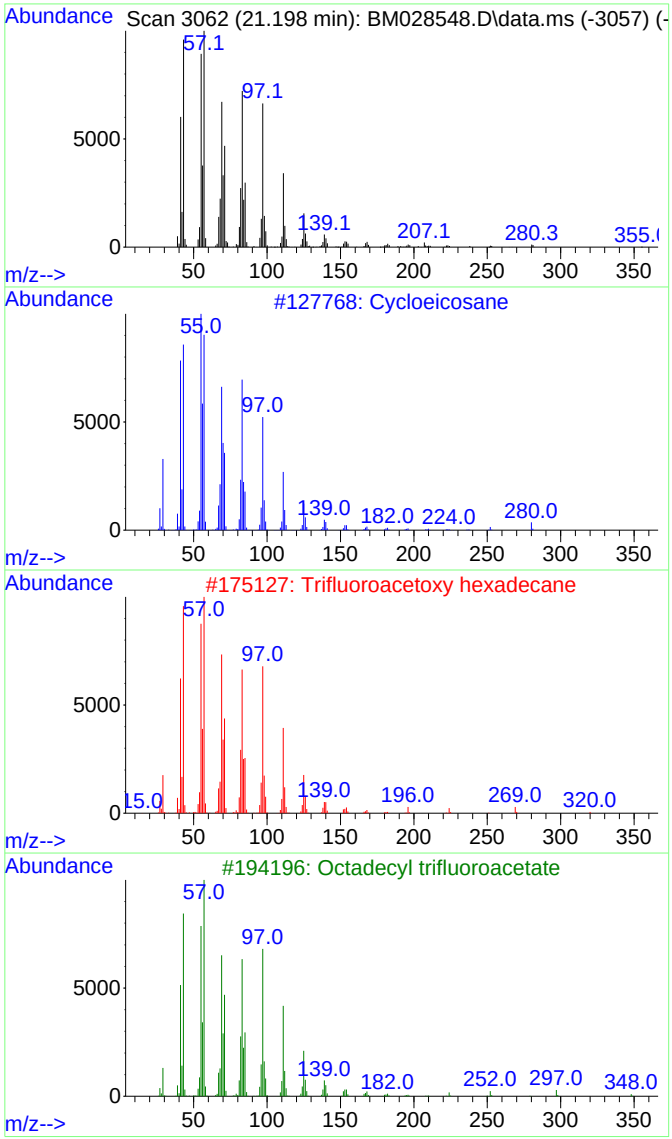
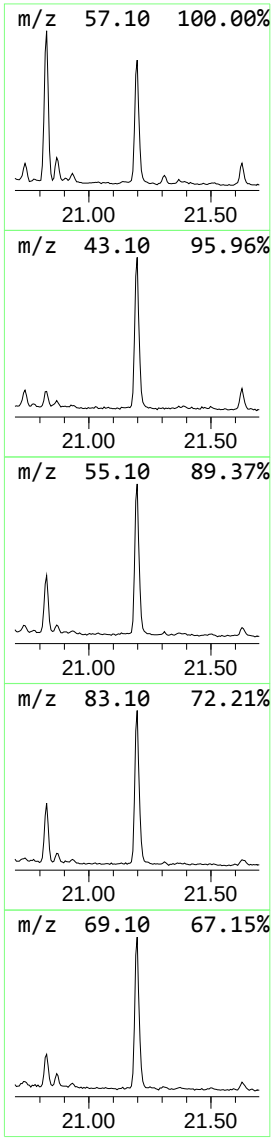
Peak Number 19 Cycloeicosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.198	24.64 ng	438839	Chrysene-d12	21.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	94
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028548.D
Acq On : 26 Jan 2021 19:33
Operator : CG/JU
Sample : M1217-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1525

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

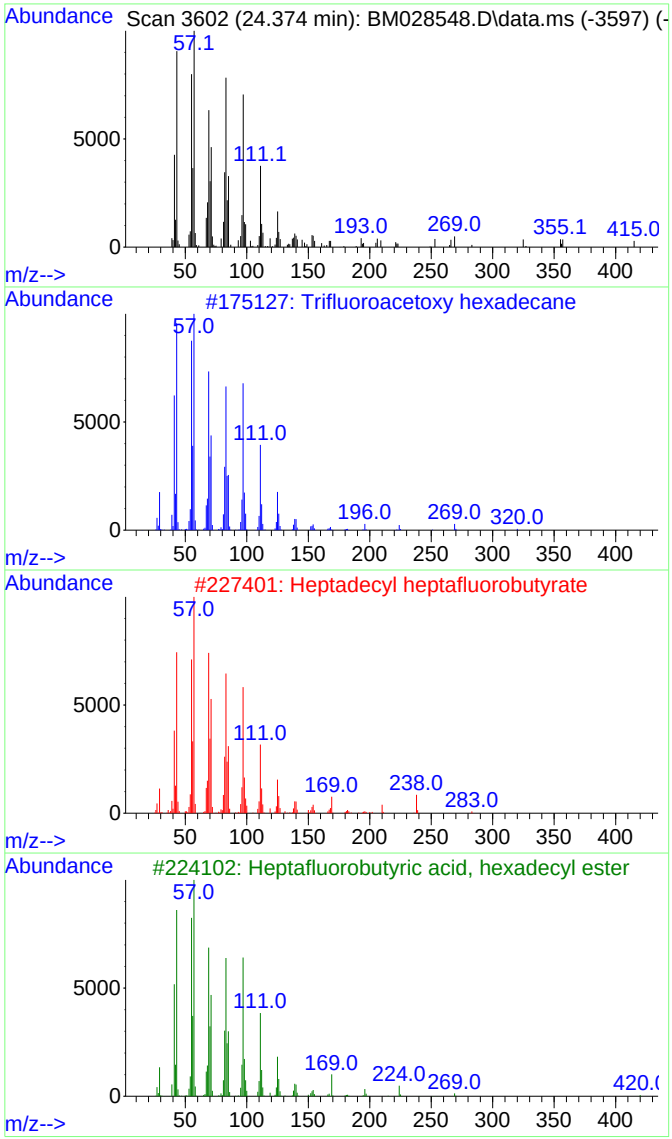
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

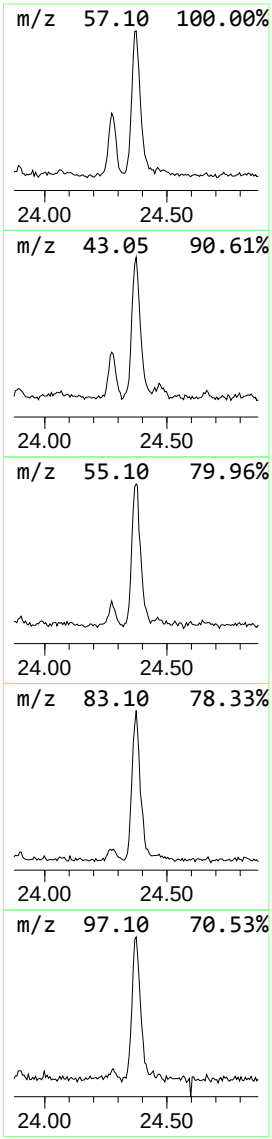
****

Peak Number 20 Trifluoroacetoxy hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.374	8.36 ng	145980	Perylene-d12	23.762

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	93
4	Octacosanol	410	C28H58O	000557-61-9	90
5	Cyclooctacosane	392	C28H56	000297-24-5	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028548.D
Acq On : 26 Jan 2021 19:33
Operator : CG/JU
Sample : M1217-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1525

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.034	3.3	ng	32809	1	7.993	201000	20.0
Ethanol, 2-butoxy-	6.034	3.1	ng	31010	1	7.993	201000	20.0
2-Propanol, 1-(...	7.522	6.6	ng	66674	1	7.993	201000	20.0
Ethane, 1-ethox...	7.581	8.0	ng	79968	1	7.993	201000	20.0
2-Propanol, 1-(...	7.769	10.9	ng	109033	1	7.993	201000	20.0
Octanoic acid	10.140	4.9	ng	66651	2	10.804	272127	20.0
1-Decene	14.275	2.8	ng	50845	3	14.633	358961	20.0
Dodecanoic acid	15.045	6.1	ng	108732	3	14.633	358961	20.0
Tridecanoic acid	15.933	4.1	ng	73939	3	14.633	358961	20.0
Pentadecane, 2,...	16.339	4.7	ng	91124	4	17.363	388999	20.0
Hexadecane, 2,6...	17.157	3.1	ng	60068	4	17.363	388999	20.0
n-Hexadecanoic ...	18.239	20.8	ng	404604	4	17.363	388999	20.0
unknown18.992	18.992	15.7	ng	305935	4	17.363	388999	20.0
4-Methyl-3,5-de...	19.074	5.6	ng	109231	4	17.363	388999	20.0
Octadecanoic acid	19.504	10.1	ng	180023	5	21.492	356220	20.0
unknown19.615	19.615	4.5	ng	80186	5	21.492	356220	20.0
Isoxazole, 3,5-...	20.621	4.2	ng	74460	5	21.492	356220	20.0
2,4,4,6,6,8,8-H...	20.827	10.3	ng	182907	5	21.492	356220	20.0
Cycloeicosane	21.198	24.6	ng	438839	5	21.492	356220	20.0
Trifluoroacetox...	24.374	8.4	ng	145980	6	23.762	349418	20.0