LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012821\
Data File : BM028592.D
Acq On : 28 Jan 2021 17:57
Operator : CG/JU
Sample : M1255-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CRT-13

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: BM028592.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.516	389	396	409	rVB	418718	621532	65.93%	8.139%
2	7.157	668	675	689	rBV	410809	662293	70.25%	8.672%
3	7.963	805	812	820	rVB	127156	196345	20.83%	2.571%
4	9.139	1004	1012	1020	rBV	256513	410126	43.50%	5.370%
5	10.775	1283	1290	1301	rVB	158547	270273	28.67%	3.539%
6	13.233	1702	1708	1715	rBV	554136	799189	84.77%	10.465%
7	14.063	1843	1849	1855	rVB	9646	11837	1.26%	0.155%
8	14.245	1876	1880	1888	rBV3	6514	10097	1.07%	0.132%
9	14.610	1936	1942	1949	rVB2	225657	318408	33.77%	4.169%
10	16.098	2189	2195	2207	rVB	414437	582405	61.78%	7.626%
11	16.333	2232	2235	2240	rVB	14108	17250	1.83%	0.226%
12	16.427	2247	2251	2255	rBV	32826	40817	4.33%	0.534%
13	16.486	2255	2261	2267	rVB2	29169	53360	5.66%	0.699%
14	16.545	2267	2271	2275	rBV2	31671	42411	4.50%	0.555%
15	16.586	2275	2278	2283	rVB	17893	23240	2.47%	0.304%
16	16.692	2294	2296	2299	rVB	10241	10628	1.13%	0.139%
17	16.745	2299	2305	2311	rVB4	28022	51759	5.49%	0.678%
18	16.810	2311	2316	2320	rBV	34880	45614	4.84%	0.597%
19	16.880	2325	2328	2335	rVB2	19504	27120	2.88%	0.355%
20	17.345	2401	2407	2411	rBV	237103	334697	35.50%	4.383%
21	17.386	2411	2414	2421	rVB	19390	26533	2.81%	0.347%
22	18.221	2549	2556	2560	rBV2	118955	160645	17.04%	2.104%
23	18.256	2560	2562	2565	rVB	11483	13211	1.40%	0.173%
24	18.404	2580	2587	2590	rBV4	10132	20550	2.18%	0.269%
25	18.439	2590	2593	2600	rVB	9231	13544	1.44%	0.177%
26	18.709	2633	2639	2644	rBV2	15267	27163	2.88%	0.356%
27	18.968	2677	2683	2688	rBV	79452	102402	10.86%	1.341%
28	19.056	2693	2698	2704	rVB	20768	26160	2.77%	0.343%
29	19.121	2705	2709	2715	rBV2	18456	27985	2.97%	0.366%
30	19.262	2729	2733	2739	rBV5	8081	14522	1.54%	0.190%
31	19.380	2748	2753	2759	rVB	65444	87375	9.27%	1.144%
32	19.486	2766	2771	2776	rBV	62223	82819	8.78%	1.084%
33	19.603	2787	2791	2798	rVB2	18408	23868	2.53%	0.313%
34	19.745	2810	2815	2822	rVB2	87878	152662	16.19%	1.999%
35	19.939	2842	2848	2858	rVB	783167	942737	100.00%	12.345%
36	20.068	2866	2870	2876	rVB3	10327	20453	2.17%	0.268%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012821\
Data File : BM028592.D
Acq On : 28 Jan 2021 17:57
Operator : CG/JU
Sample : M1255-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CRT-13

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	20.127	2877	2880	2886	rVB	12296	17755	1.88%	0.232%
38	20.203	2888	2893	2896	rBV6	13278	27617	2.93%	0.362%
39	20.339	2912	2916	2919	rBV3	8891	14050	1.49%	0.184%
40	20.392	2921	2925	2928	rVV	12694	16528	1.75%	0.216%
41	20.527	2944	2948	2951	rBV2	16480	23692	2.51%	0.310%
42	20.568	2952	2955	2958	rVV2	20713	30062	3.19%	0.394%
43	20.603	2958	2961	2967	rVB	27709	40900	4.34%	0.536%
44	20.809	2992	2996	3000	rBV	101056	113158	12.00%	1.482%
45	20.856	3001	3004	3007	rVB	19252	21472	2.28%	0.281%
46	21.174	3054	3058	3063	rBV2	124254	162420	17.23%	2.127%
47	21.480	3103	3110	3114	rBV2	312384	469596	49.81%	6.149%
48	21.515	3114	3116	3122	rVB	57053	66880	7.09%	0.876%
49	23.744	3489	3495	3501	rBV2	195154	360629	38.25%	4.722%

Sum of corrected areas: 7636789

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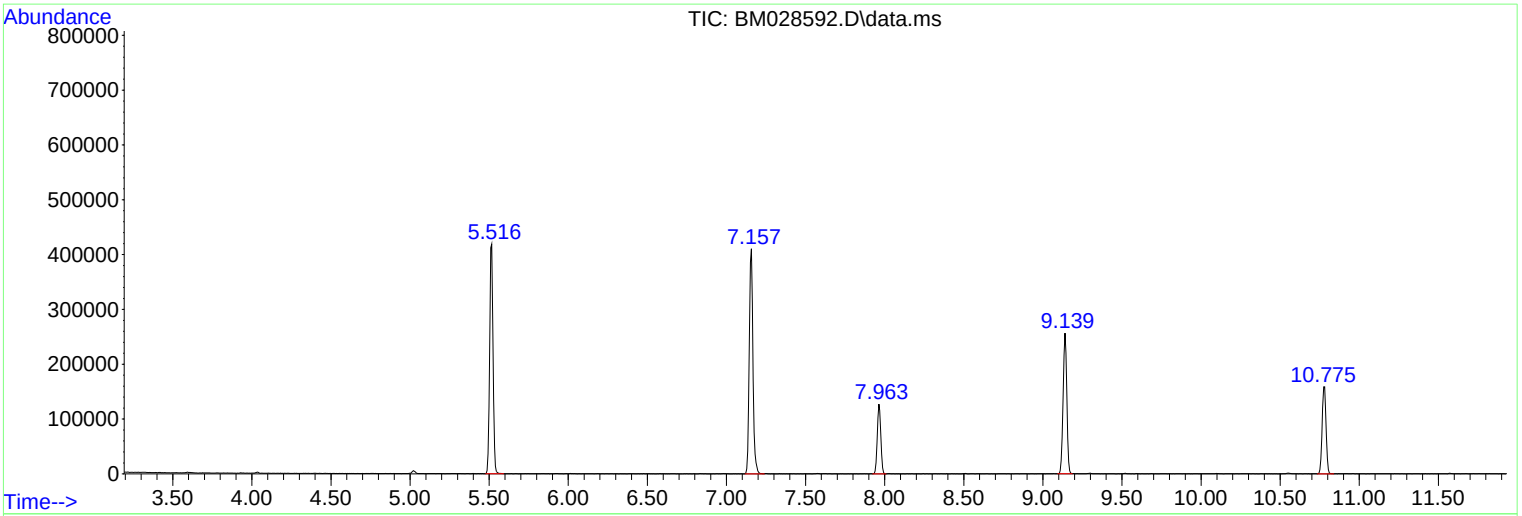
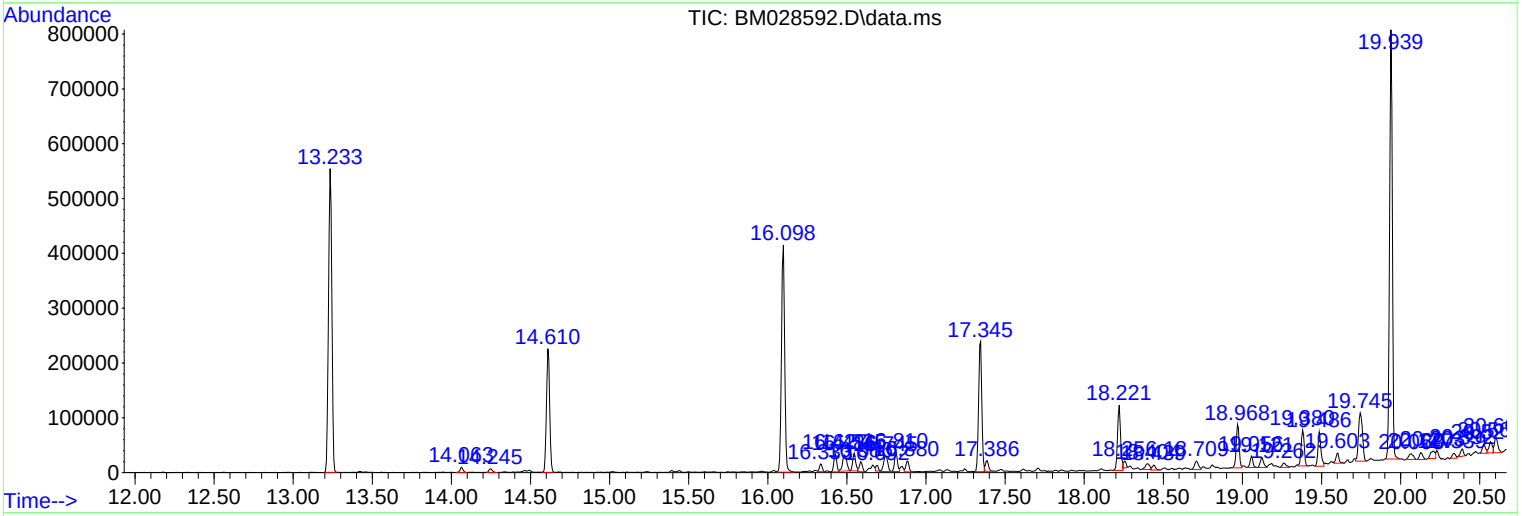
Misc :
ALS Vial : 11 Sample Multiplier: 1

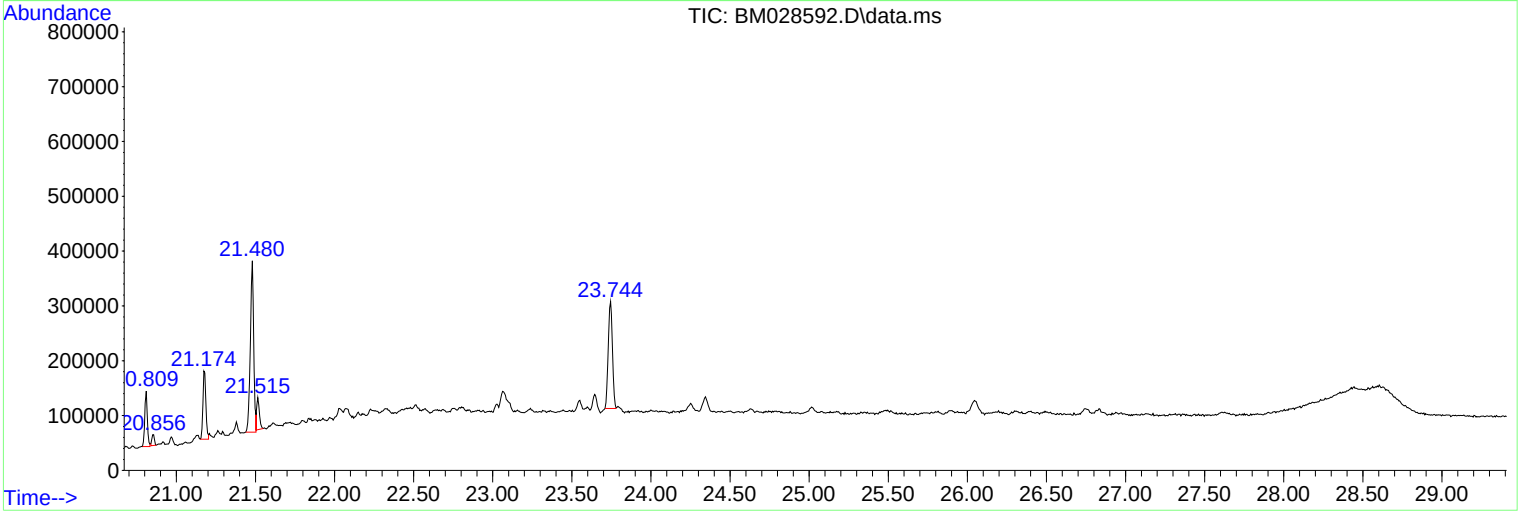
Instrument :
BNA_M
ClientSampleId :
CRT-13

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\BM012821\
Data File : BM028592.D
Acq On : 28 Jan 2021 17:57
Operator : CG/JU
Sample : M1255-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CRT-13

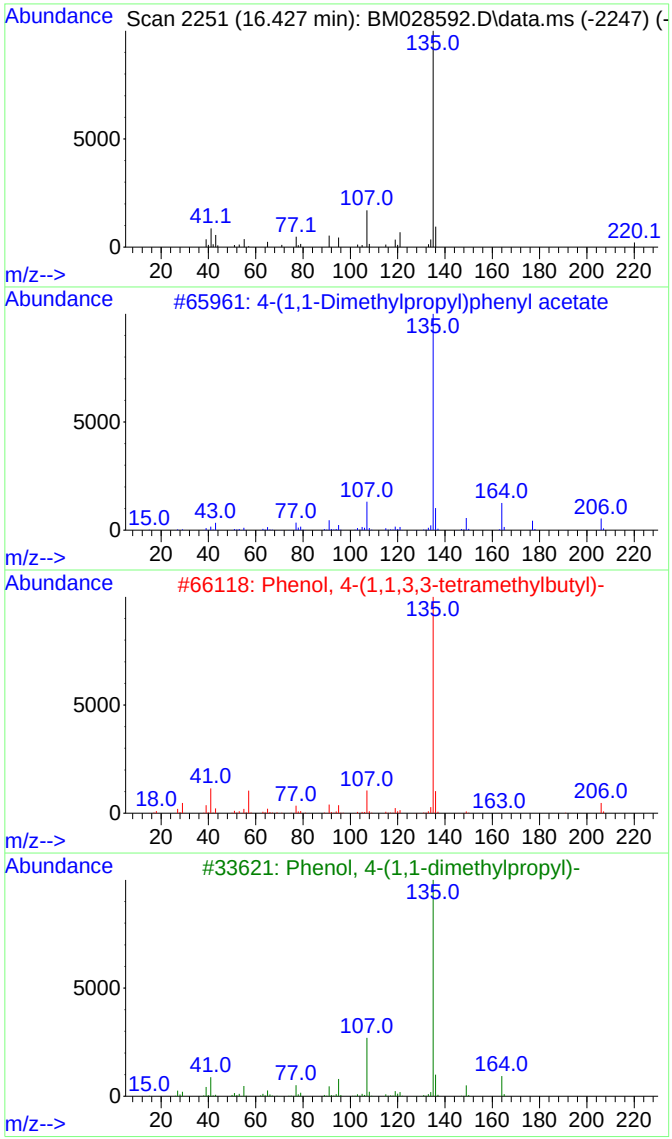
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

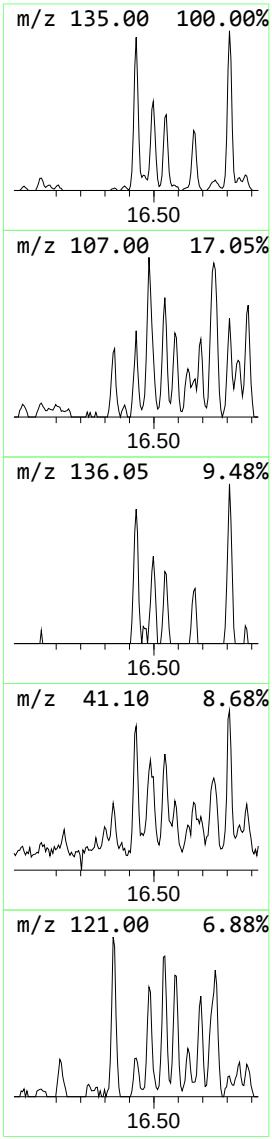
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 4-(1,1-Dimethylpropyl)pheny... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.427	2.44 ng	40817	Phenanthrene-d10	17.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	83
2	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	78
3	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	78
4	Hexestrol	270	C18H22O2	000084-16-2	64
5	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	000499-75-2	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012821\
Data File : BM028592.D
Acq On : 28 Jan 2021 17:57
Operator : CG/JU
Sample : M1255-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CRT-13

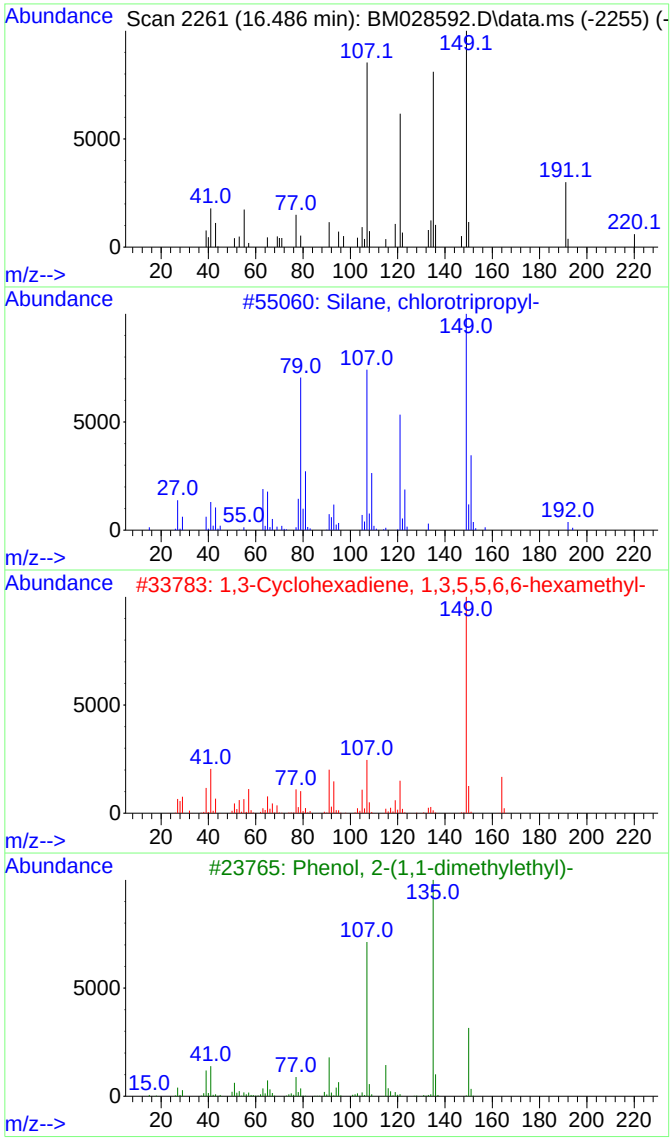
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

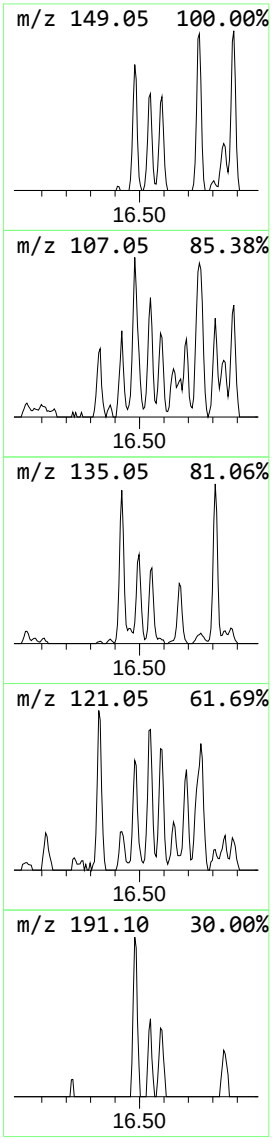
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Silane, chlorotripropyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.486	3.19 ng	53360	Phenanthrene-d10	17.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, chlorotripropyl-	192	C9H21ClSi	000995-25-5	53
2	1,3-Cyclohexadiene, 1,3,5,5,6,6-...	164	C12H20	1000150-39-4	47
3	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	46
4	Acetamide, N-(4-methylphenyl)-	149	C9H11NO	000103-89-9	46
5	Hexestrol	270	C18H22O2	005635-50-7	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012821\
Data File : BM028592.D
Acq On : 28 Jan 2021 17:57
Operator : CG/JU
Sample : M1255-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CRT-13

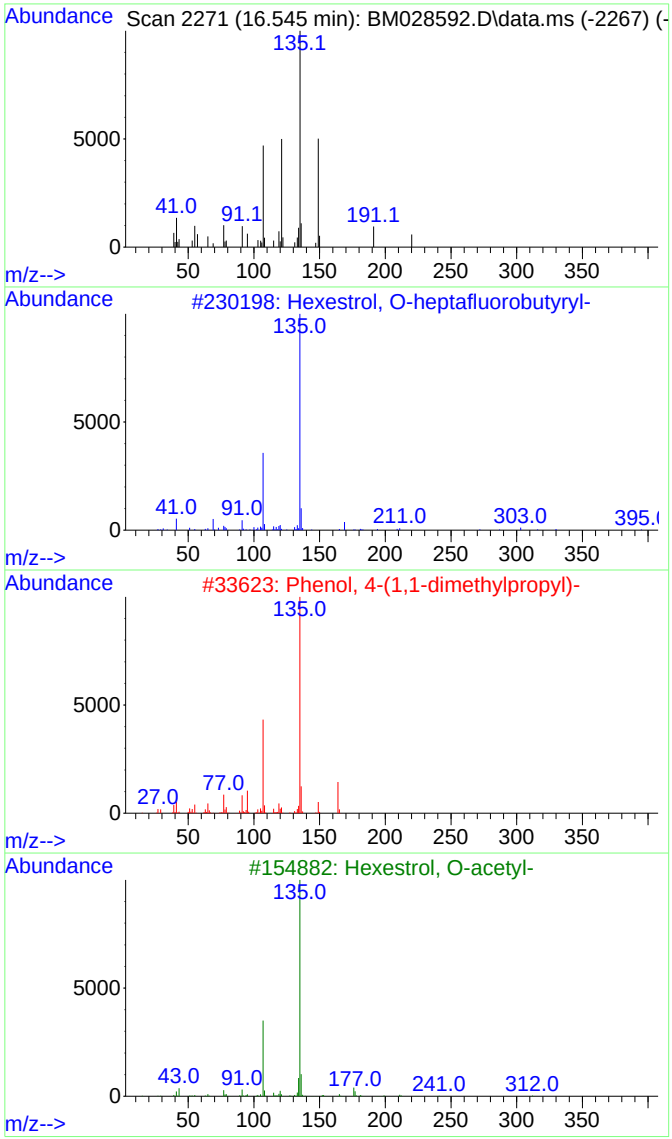
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

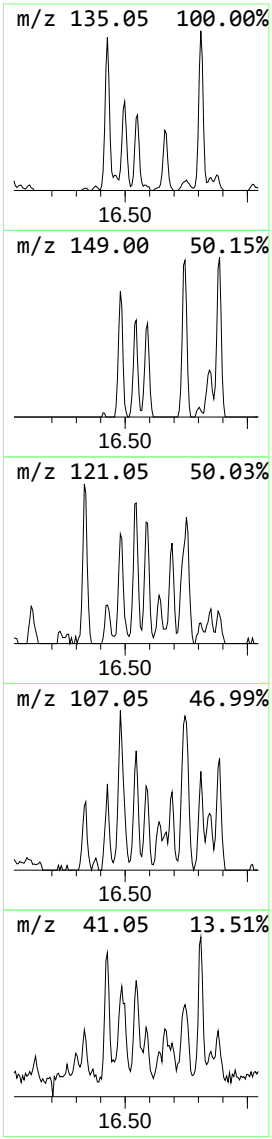
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Hexestrol, O-heptafluorobut... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.545	2.53 ng	42411	Phenanthrene-d10	17.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexestrol, O-heptafluorobutyryl-	466	C22H21F7O3	1000365-31-9	50
2	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	50
3	Hexestrol, O-acetyl-	312	C20H24O3	1000374-87-8	50
4	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	50
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012821\
Data File : BM028592.D
Acq On : 28 Jan 2021 17:57
Operator : CG/JU
Sample : M1255-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CRT-13

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

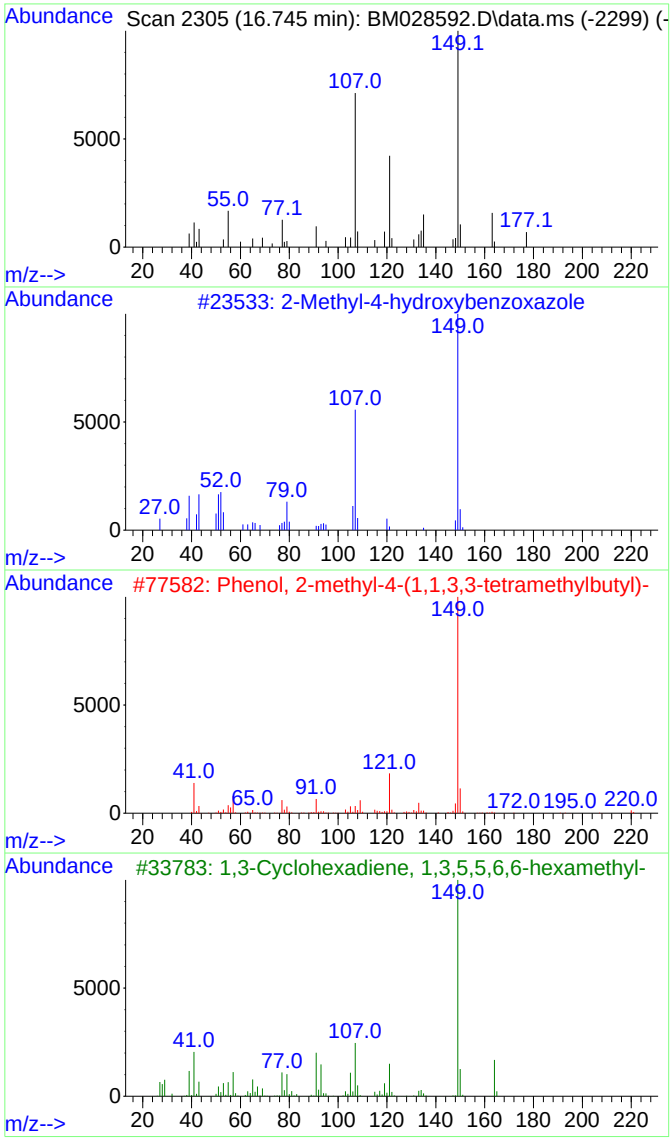
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

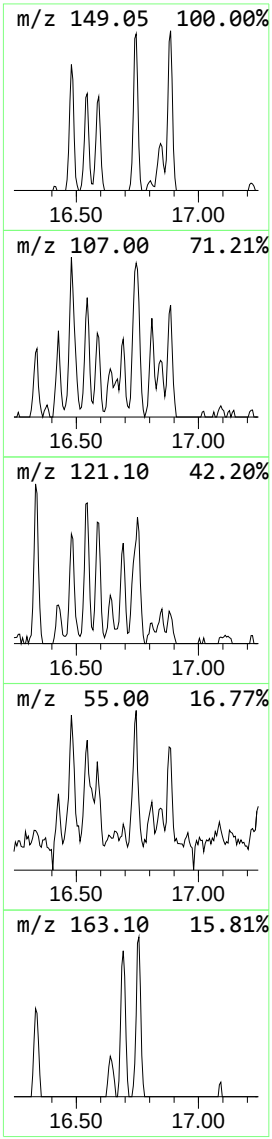
****

Peak Number 4 2-Methyl-4-hydroxybenzoxazole Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.745	3.09 ng	51759	Phenanthrene-d10	17.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	59
2	Phenol, 2-methyl-4-(1,1,3,3-tetr...	220	C15H24O	002219-84-3	47
3	1,3-Cyclohexadiene, 1,3,5,5,6,6-...	164	C12H20	1000150-39-4	45
4	3',4'-Formoxylidide	149	C9H11NO	006639-60-7	43
5	2H-Indol-2-one, 1,3-dihydro-5-hy...	149	C8H7NO2	003416-18-0	43





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Sample : M1255-06
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CRT-13

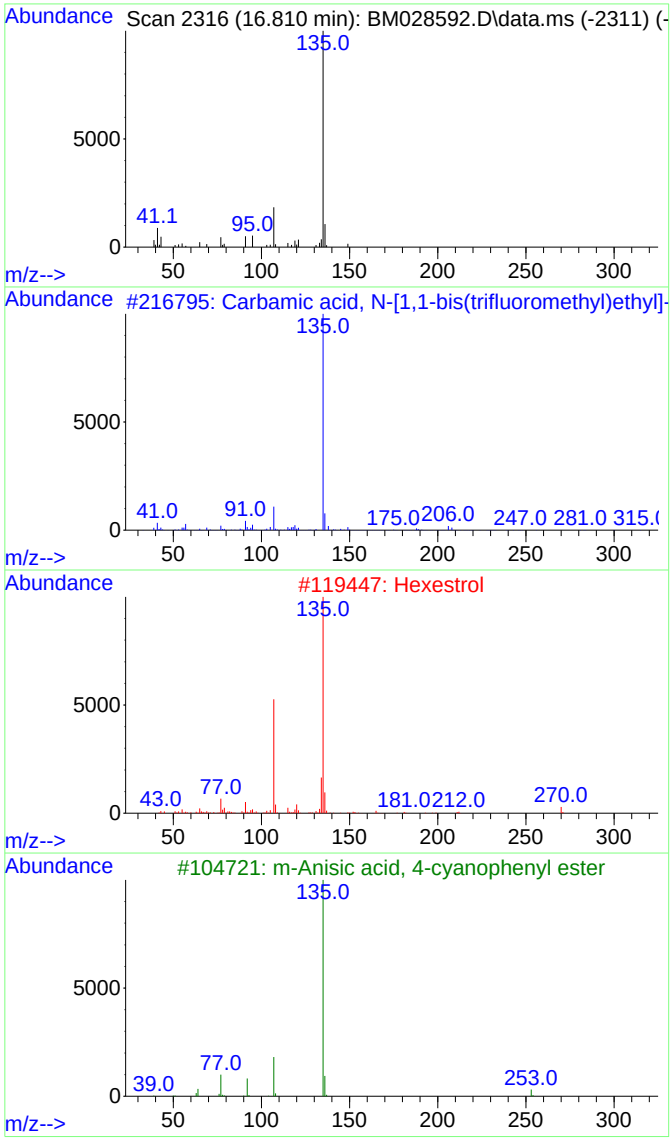
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

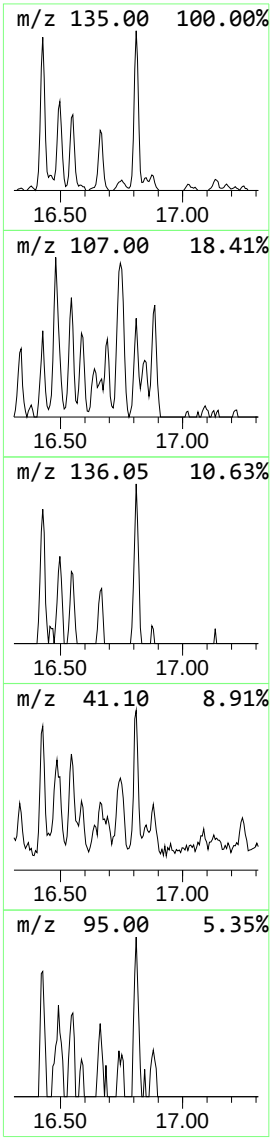
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Carbamic acid, N-[1,1-bis(t... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.810	2.73 ng	45614	Phenanthrene-d10	17.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbamic acid, N-[1,1-bis(triflu...	413	C19H25F6NO2	296242-69-8	78
2	Hexestrol	270	C18H22O2	000084-16-2	50
3	m-Anisic acid, 4-cyanophenyl ester	253	C15H11NO3	1000307-80-2	50
4	1,3-Benzenediol, o-(2-furoyl)-o'...	338	C19H14O6	1000330-77-5	50
5	4-Methoxybenzoic acid, 2,6-dimet...	422	C19H16F6O4	1000304-50-0	50





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ALS Vial : 11 Sample Multiplier: 1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

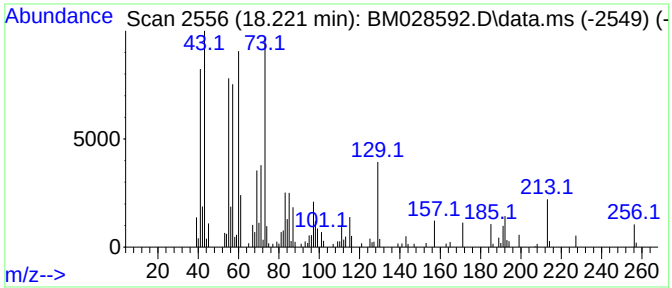
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

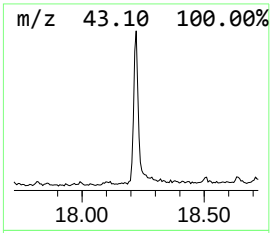
****

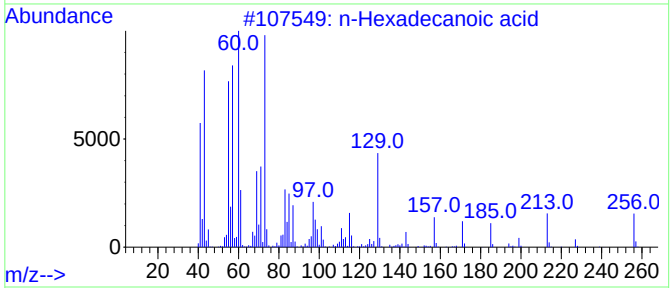
Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

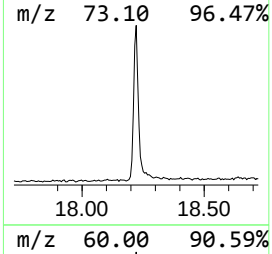
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.221	9.60 ng	160645	Phenanthrene-d10	17.345

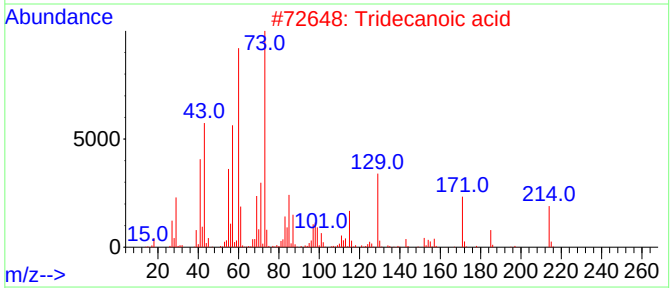
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	Undecanoic acid	186	C11H22O2	000112-37-8	53

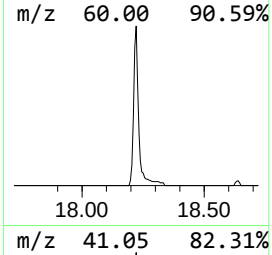


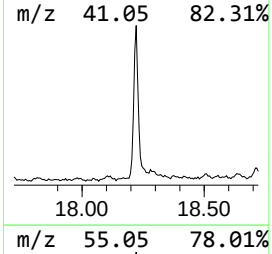


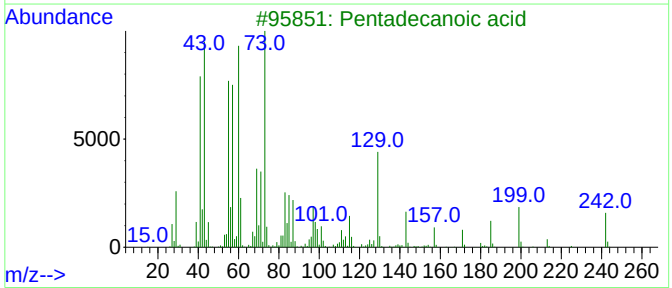


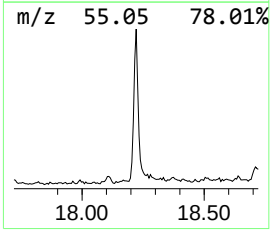












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Data File : BM028592.D
Acq On : 28 Jan 2021 17:57
Operator : CG/JU
Sample : M1255-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CRT-13

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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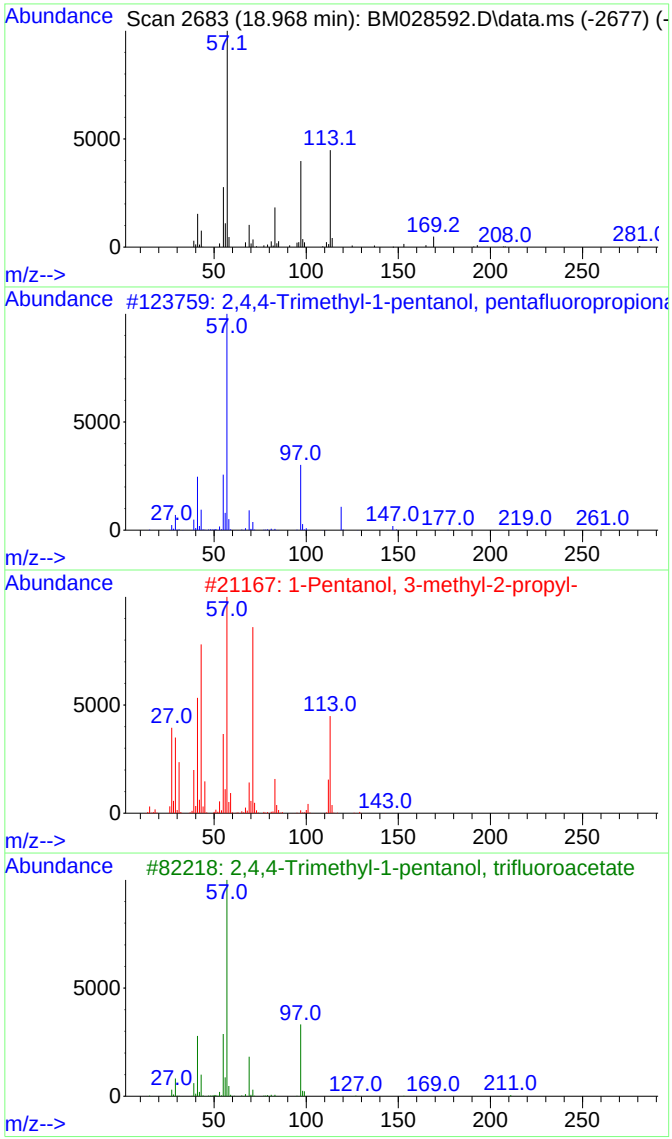
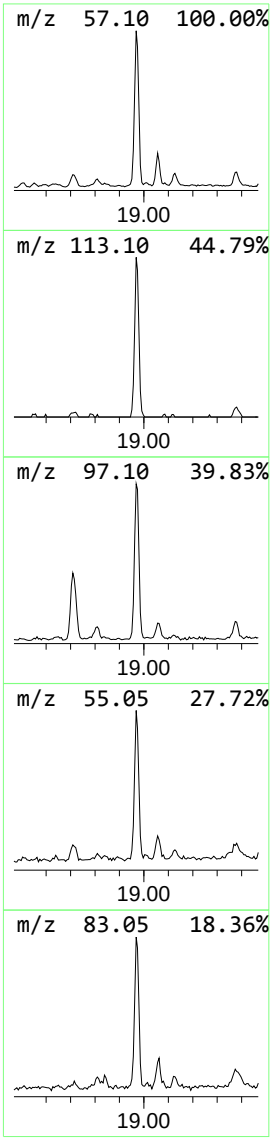
Peak Number 7 unknown18.968 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.968	6.12 ng	102402	Phenanthrene-d10	17.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	43
2	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	40
3	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	38
4	Octane, 2-bromo-	192	C8H17Br	000557-35-7	38
5	Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012821\
Data File : BM028592.D
Acq On : 28 Jan 2021 17:57
Operator : CG/JU
Sample : M1255-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

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ClientSampleId : CRT-13

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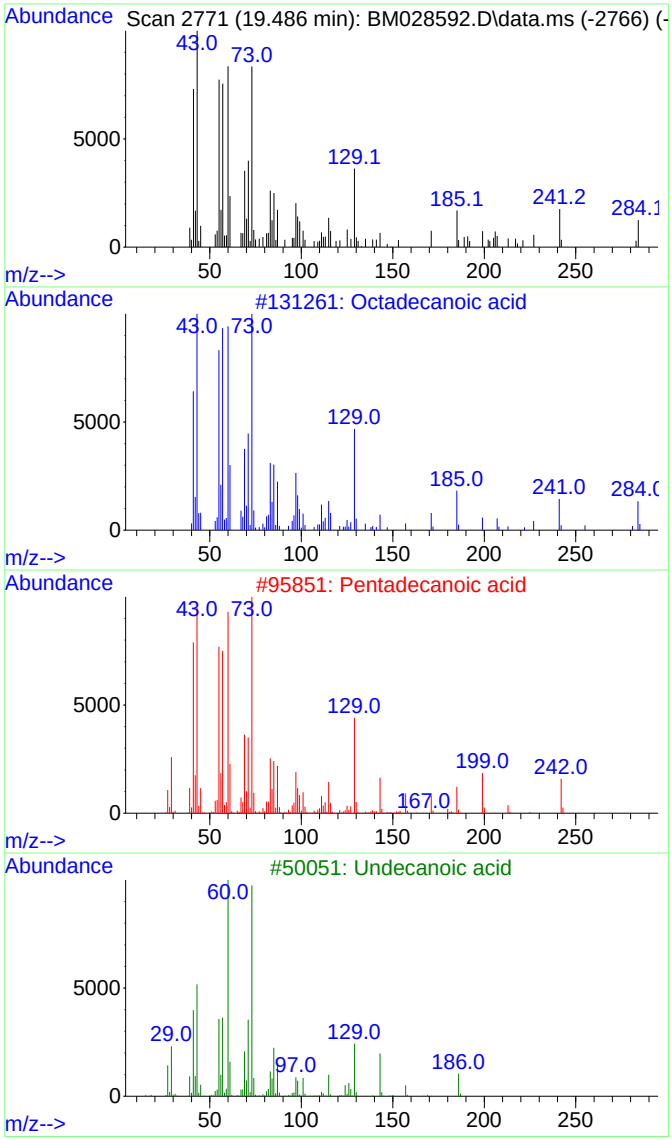
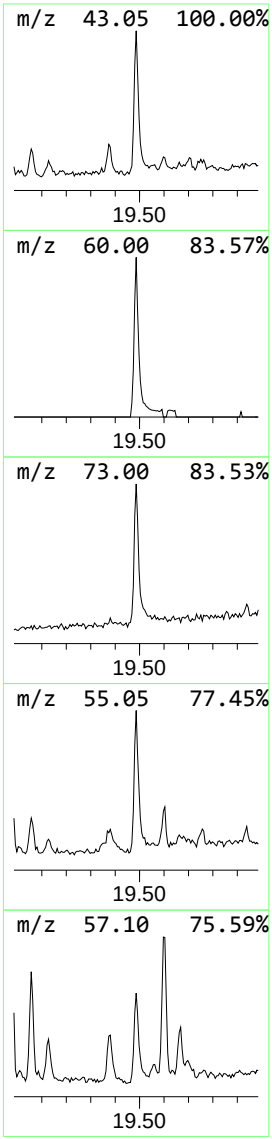
Peak Number 8 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.486	3.53 ng	82819	Chrysene-d12	21.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Undecanoic acid	186	C11H22O2	000112-37-8	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58





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Data File : BM028592.D
Acq On : 28 Jan 2021 17:57
Operator : CG/JU
Sample : M1255-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CRT-13

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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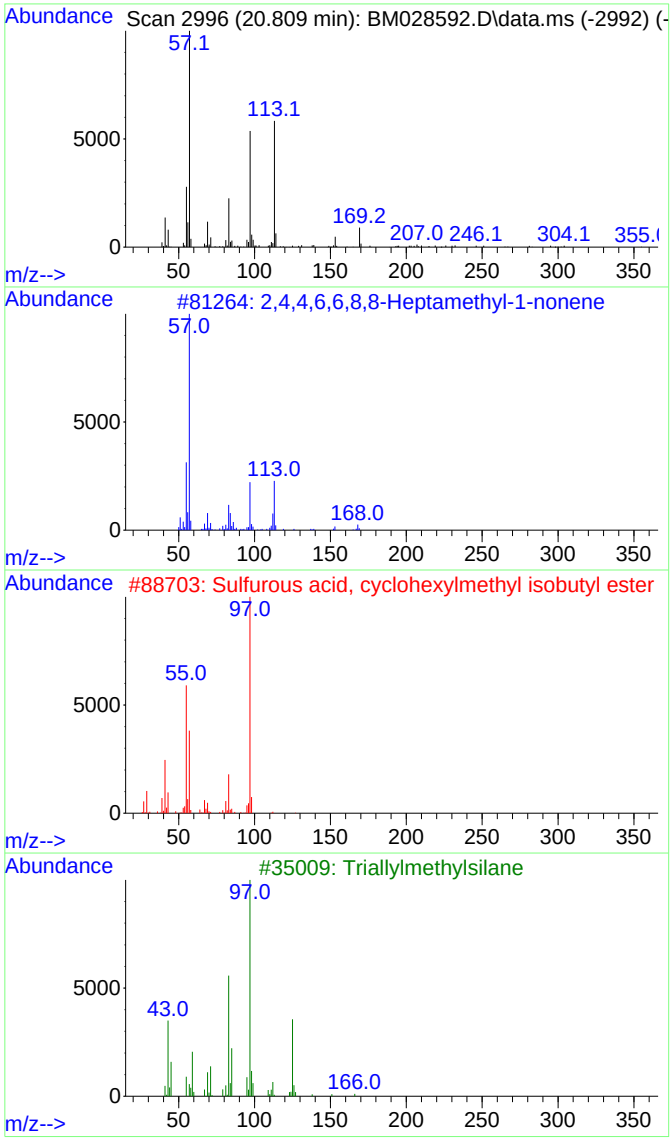
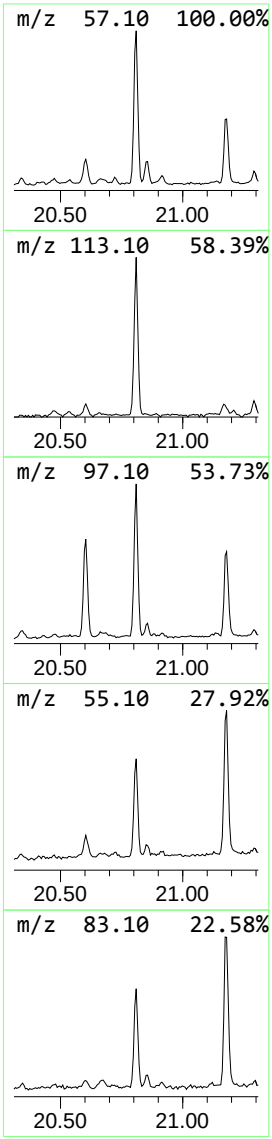
Peak Number 9 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.809	4.82 ng	113158	Chrysene-d12	21.480

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	78
2	Sulfurous acid, cyclohexylmethyl...	234	C11H22O3S	1000309-21-3	25
3	Triallylmethylsilane	166	C10H18Si	001112-91-0	25
4	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	22
5	Silane, butyldichloromethyl-	170	C5H12Cl2Si	018147-23-4	22





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Sample : M1255-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CRT-13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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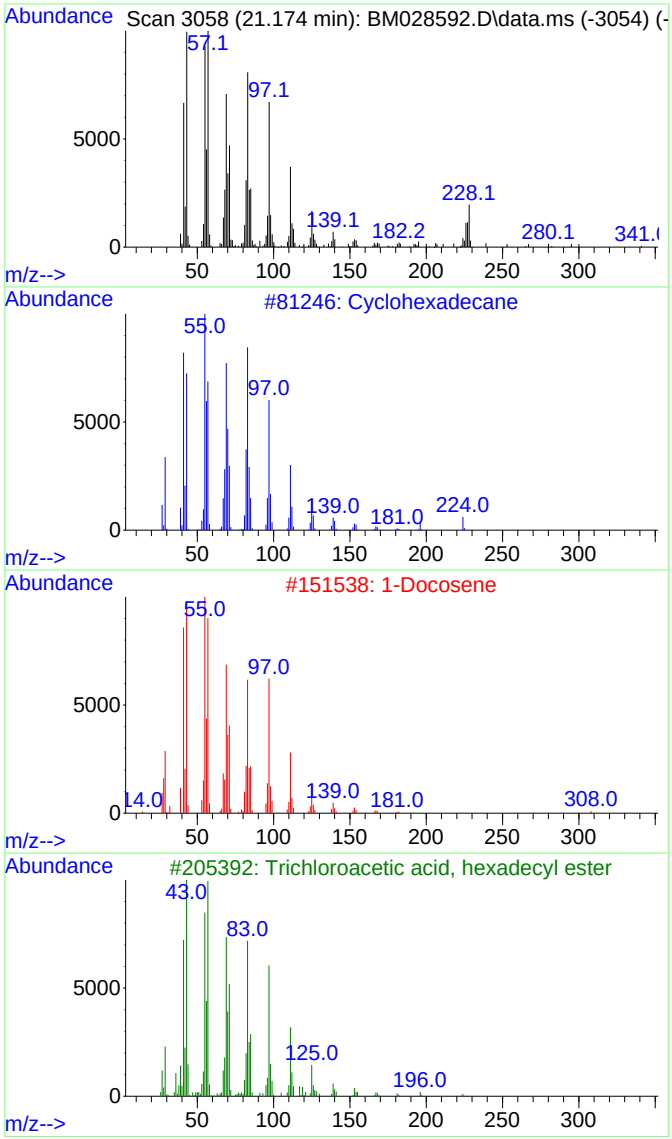
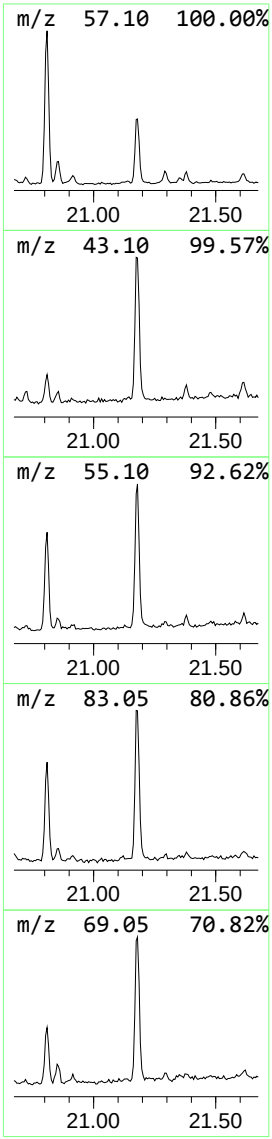
Peak Number 10 Cyclohexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.174	6.92 ng	162420	Chrysene-d12	21.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	97
2	1-Docosene	308	C22H44	001599-67-3	93
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012821\
Data File : BM028592.D
Acq On : 28 Jan 2021 17:57
Operator : CG/JU
Sample : M1255-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CRT-13

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
4-(1,1-Dimethyl...	16.427	2.4	ng	40817	4	17.345	334697	20.0
Silane, chlorot...	16.486	3.2	ng	53360	4	17.345	334697	20.0
Hexestrol, O-he...	16.545	2.5	ng	42411	4	17.345	334697	20.0
2-Methyl-4-hydr...	16.745	3.1	ng	51759	4	17.345	334697	20.0
Carbamic acid, ...	16.810	2.7	ng	45614	4	17.345	334697	20.0
n-Hexadecanoic ...	18.221	9.6	ng	160645	4	17.345	334697	20.0
unknown18.968	18.968	6.1	ng	102402	4	17.345	334697	20.0
Octadecanoic acid	19.486	3.5	ng	82819	5	21.480	469596	20.0
2,4,4,6,6,8,8-H...	20.809	4.8	ng	113158	5	21.480	469596	20.0
Cyclohexadecane	21.174	6.9	ng	162420	5	21.480	469596	20.0