LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012821\
Data File : BM028598.D
Acq On : 28 Jan 2021 21:34
Operator : CG/JU
Sample : M1241-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : FACILITY-1

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: BM028598.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.746	90	95	103	rVB	6242	9835	2.47%	0.270%
2	4.381	198	203	213	rBV	268877	367038	92.05%	10.095%
3	5.016	306	311	319	rBV	151574	203704	51.09%	5.603%
4	7.157	670	675	681	rBV	10087	15946	4.00%	0.439%
5	7.963	805	812	819	rBV	129167	196007	49.15%	5.391%
6	8.634	920	926	931	rVB2	4466	7185	1.80%	0.198%
7	9.139	1006	1012	1017	rBV	40138	63359	15.89%	1.743%
8	10.780	1284	1291	1296	rBV	158506	258846	64.91%	7.119%
9	10.828	1296	1299	1304	rVB	8014	11232	2.82%	0.309%
10	12.180	1523	1529	1533	rBV	3212	4487	1.13%	0.123%
11	12.439	1569	1573	1577	rBV	2651	4112	1.03%	0.113%
12	13.233	1702	1708	1714	rVB	103864	142378	35.71%	3.916%
13	13.421	1735	1740	1747	rBV2	5266	8253	2.07%	0.227%
14	14.074	1845	1851	1855	rVB3	2854	5001	1.25%	0.138%
15	14.463	1909	1917	1919	rBV3	2304	4748	1.19%	0.131%
16	14.492	1919	1922	1927	rVB2	6238	8274	2.07%	0.228%
17	14.610	1935	1942	1949	rVB2	213167	314638	78.91%	8.654%
18	14.674	1949	1953	1958	rVB2	4473	5905	1.48%	0.162%
19	15.004	2004	2009	2015	rBV2	4338	7119	1.79%	0.196%
20	15.439	2079	2083	2088	rBV	6046	7471	1.87%	0.205%
21	15.657	2115	2120	2126	rBV2	5526	8625	2.16%	0.237%
22	16.298	2225	2229	2232	rBV2	6959	9969	2.50%	0.274%
23	17.086	2358	2363	2368	rBV2	6958	8548	2.14%	0.235%
24	17.139	2368	2372	2375	rBV3	3015	5305	1.33%	0.146%
25	17.345	2401	2407	2411	rBV	241390	336768	84.46%	9.262%
26	17.386	2411	2414	2420	rVB	54642	68592	17.20%	1.887%
27	17.474	2425	2429	2437	rVV	11666	17174	4.31%	0.472%
28	17.745	2470	2475	2482	rBV4	4582	7692	1.93%	0.212%
29	17.815	2482	2487	2492	rBV2	5984	8373	2.10%	0.230%
30	17.992	2514	2517	2522	rVB2	7999	9788	2.45%	0.269%
31	18.215	2550	2555	2560	rBV2	35237	59689	14.97%	1.642%
32	18.262	2560	2563	2569	rVB2	11180	16657	4.18%	0.458%
33	18.409	2583	2588	2592	rBV3	8559	17728	4.45%	0.488%
34	18.509	2601	2605	2609	rBV2	7509	10075	2.53%	0.277%
35	18.709	2636	2639	2643	rVB2	5034	6383	1.60%	0.176%
36	18.756	2645	2647	2651	rVB5	4902	5414	1.36%	0.149%

LSC Area Percent Report

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

37	19.127	2706	2710	2713	rBV3	28512	36373	9.12%	1.000%
38	19.156	2713	2715	2724	rVB4	20775	28193	7.07%	0.775%
39	19.386	2744	2754	2767	rBV	91531	224990	56.42%	6.188%
40	19.486	2768	2771	2776	rVV2	20213	28216	7.08%	0.776%
41	19.621	2791	2794	2797	rBV4	9133	13070	3.28%	0.359%
42	19.709	2806	2809	2811	rBV2	11772	13286	3.33%	0.365%
43	19.745	2811	2815	2824	rVB	58944	82101	20.59%	2.258%
44	19.939	2843	2848	2853	rVB	163407	193925	48.63%	5.334%
45	21.180	3057	3059	3063	rVB2	37286	35392	8.88%	0.973%
46	21.480	3105	3110	3115	rBV	282955	398753	100.00%	10.967%
47	23.750	3491	3496	3503	rVB2	191846	339317	85.09%	9.332%

Sum of corrected areas: 3635934

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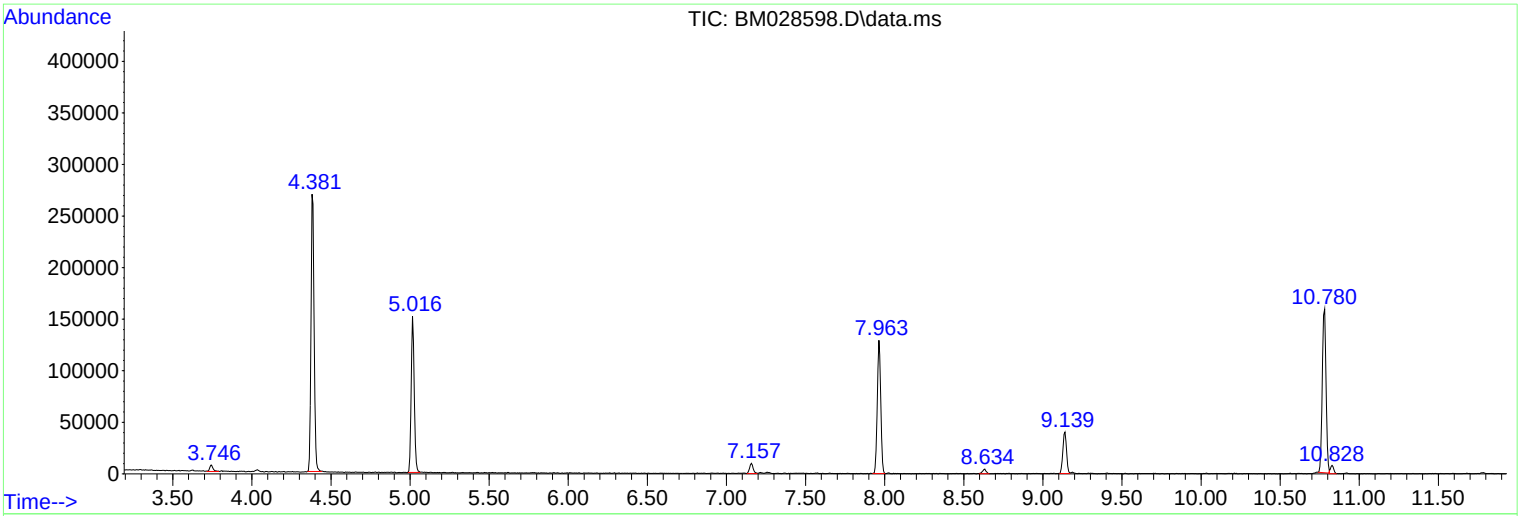
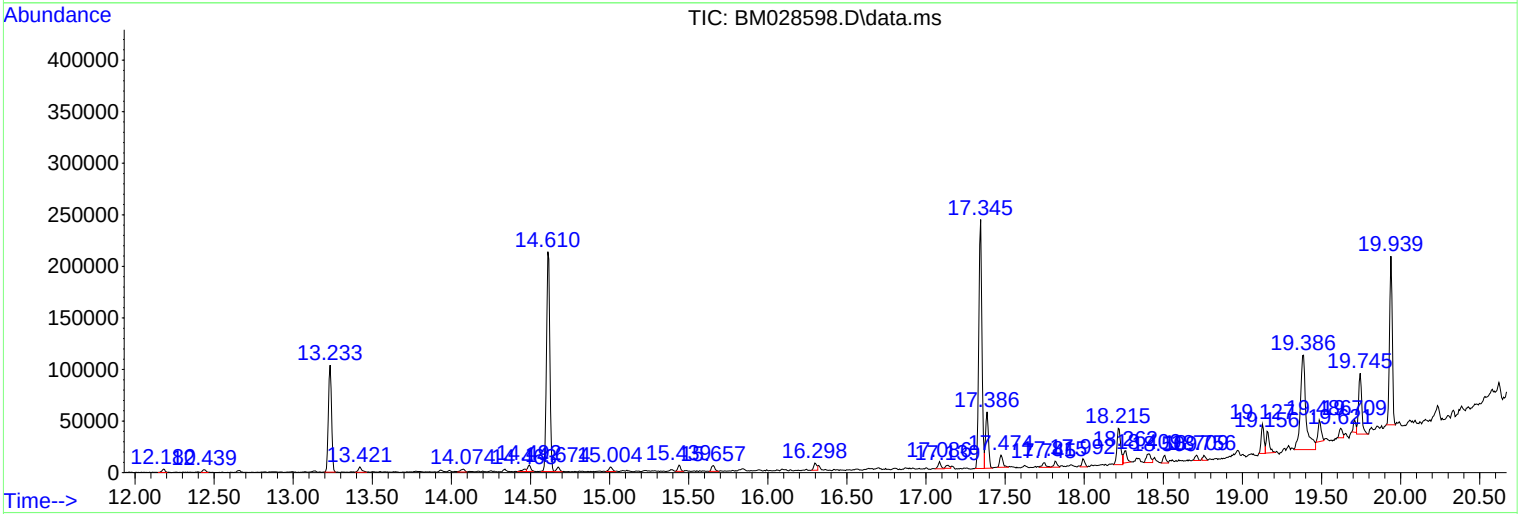
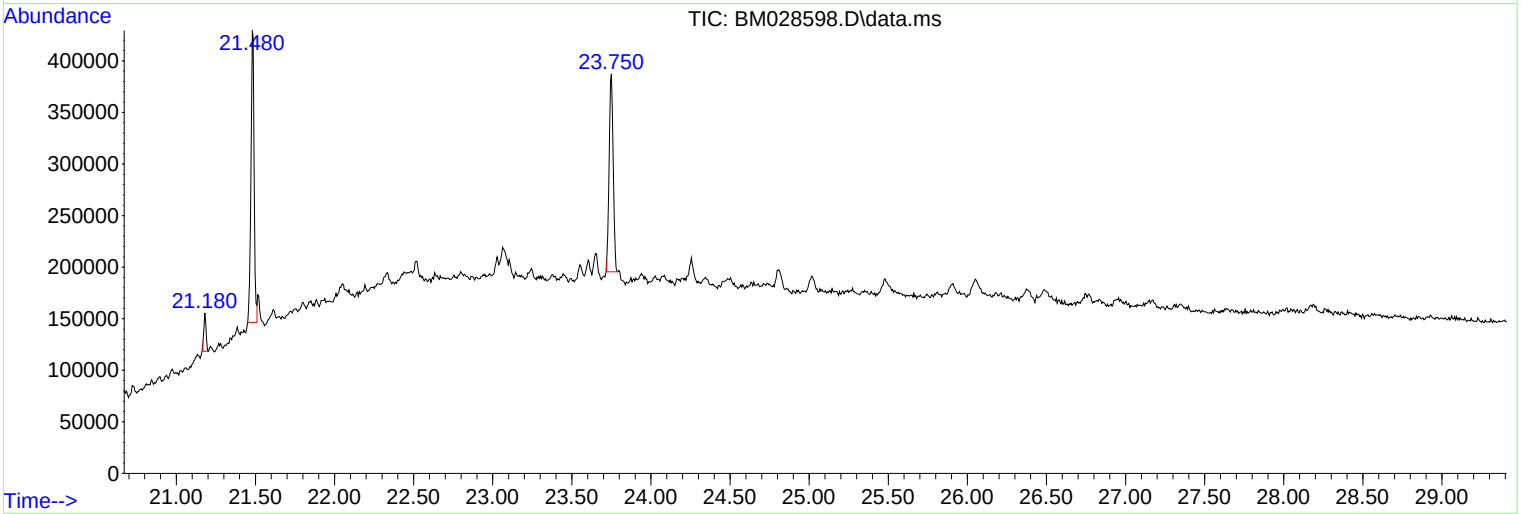
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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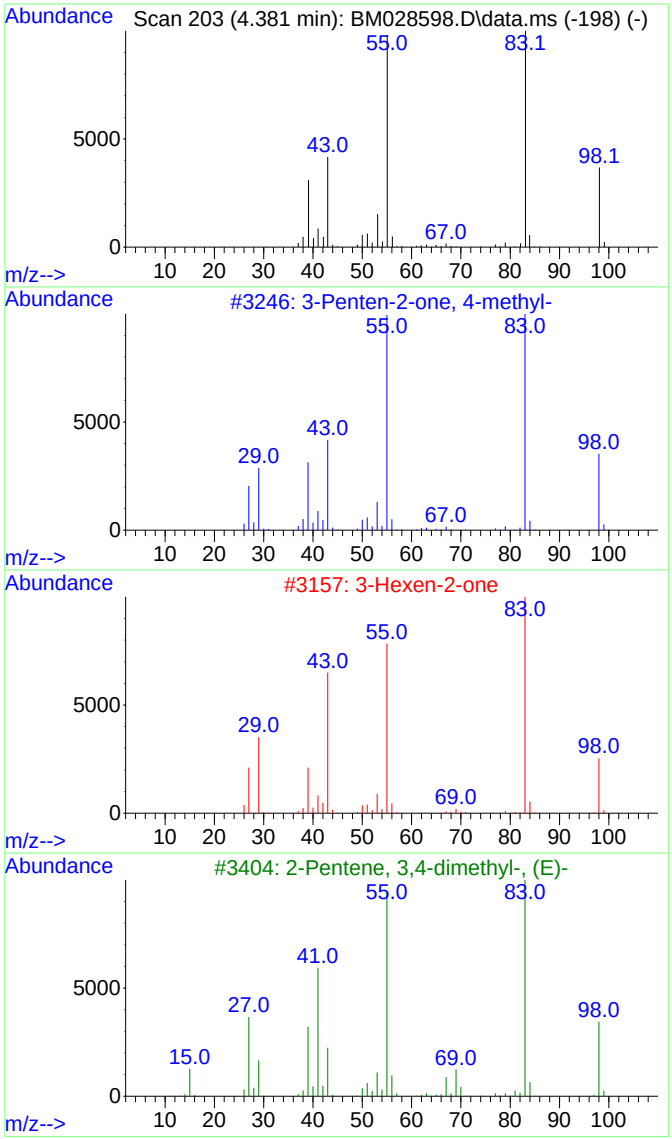
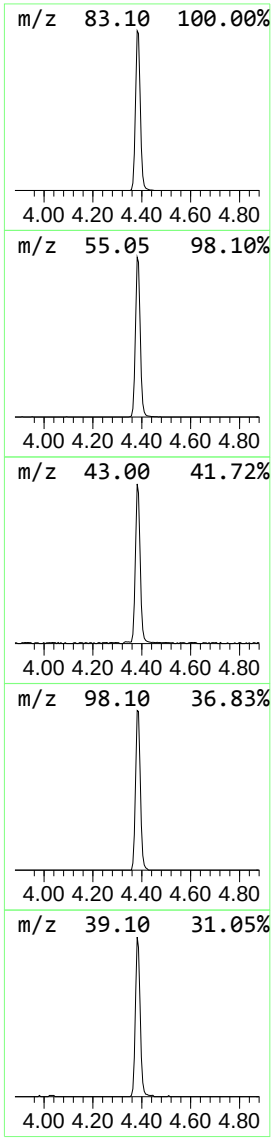
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.381	37.45 ng	367038	1,4-Dichlorobenzene-d4	7.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





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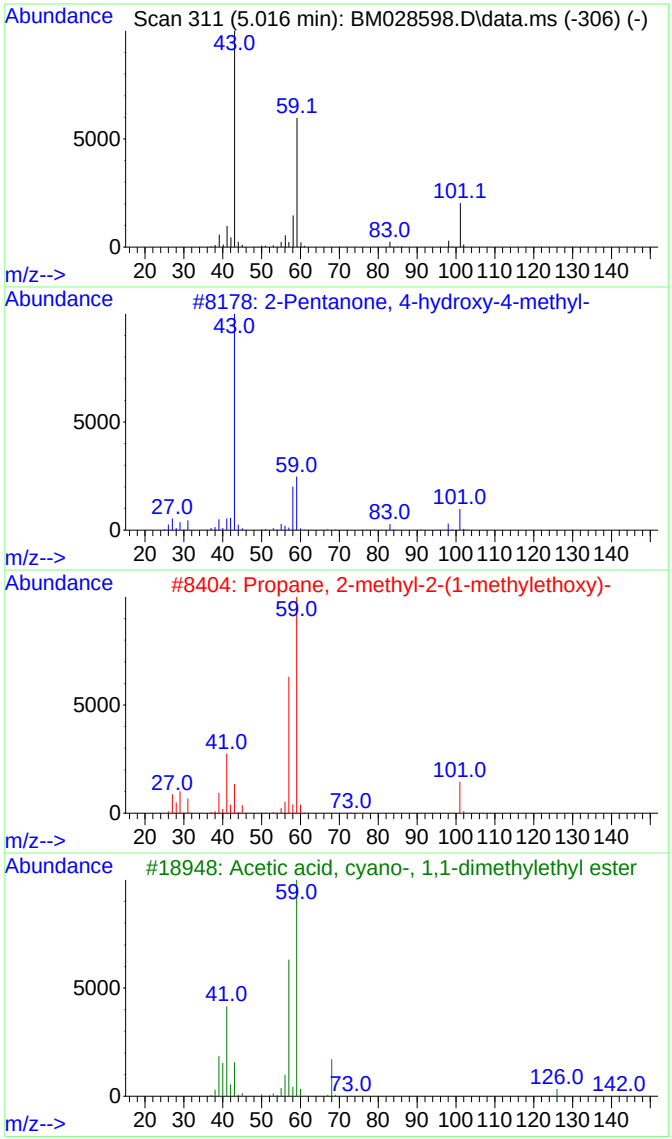
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

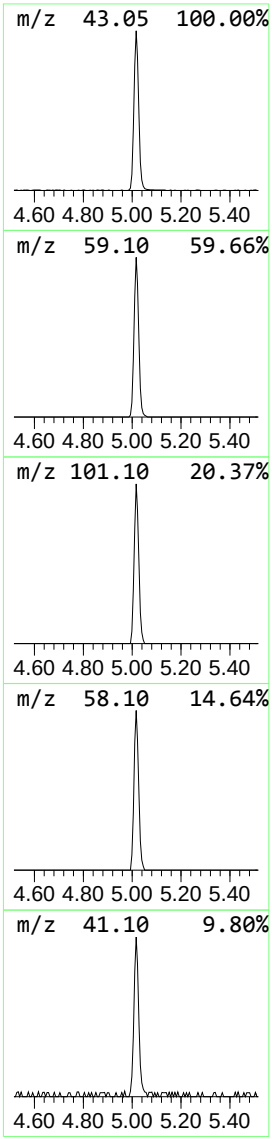
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	20.79 ng	203704	1,4-Dichlorobenzene-d4	7.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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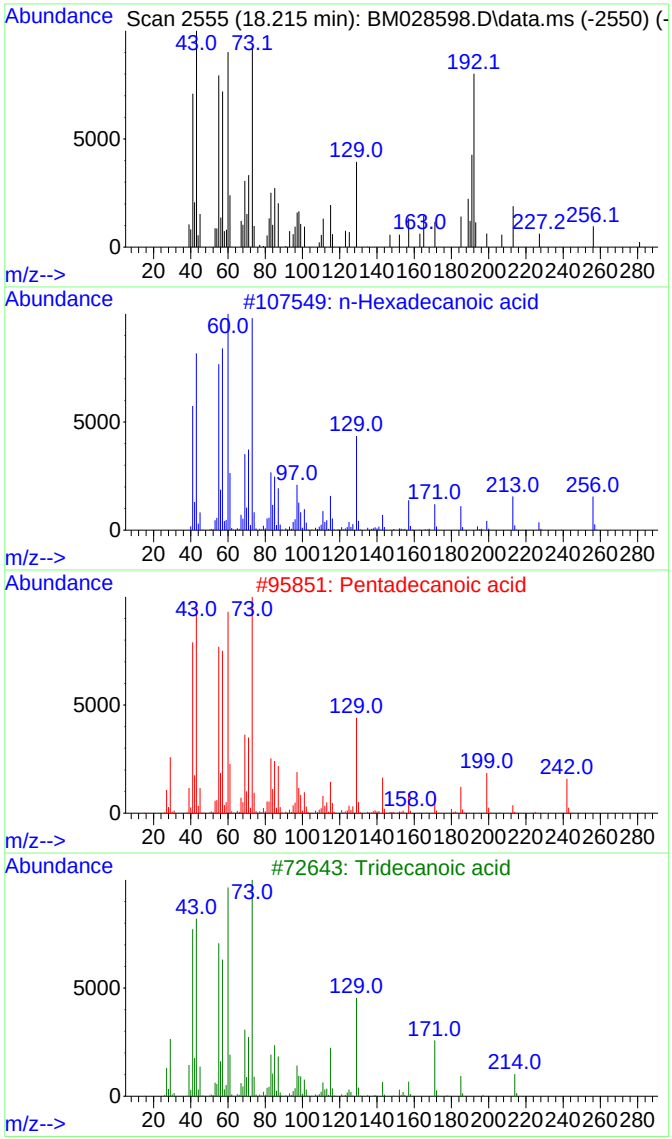
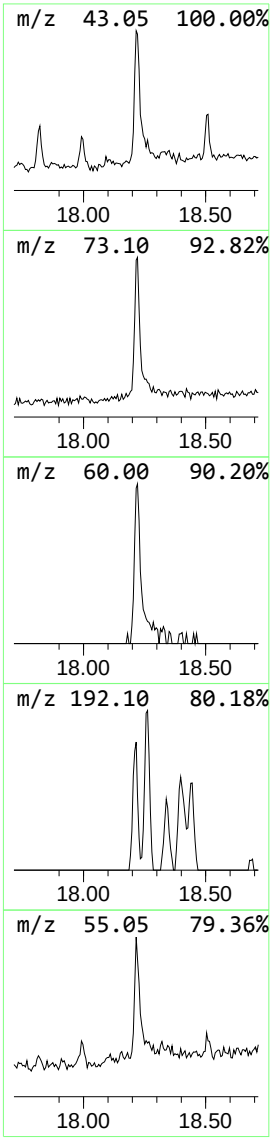
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.215	3.54 ng	59689	Phenanthrene-d10	17.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	55
3	Tridecanoic acid	214	C13H26O2	000638-53-9	49
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	30





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

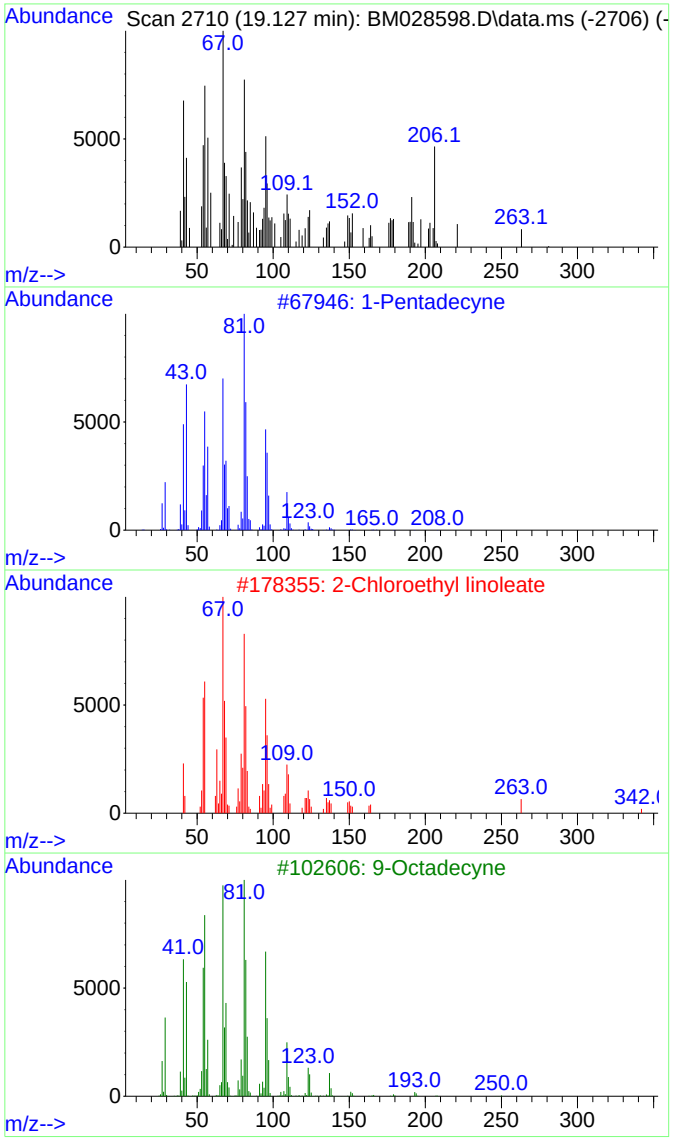
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

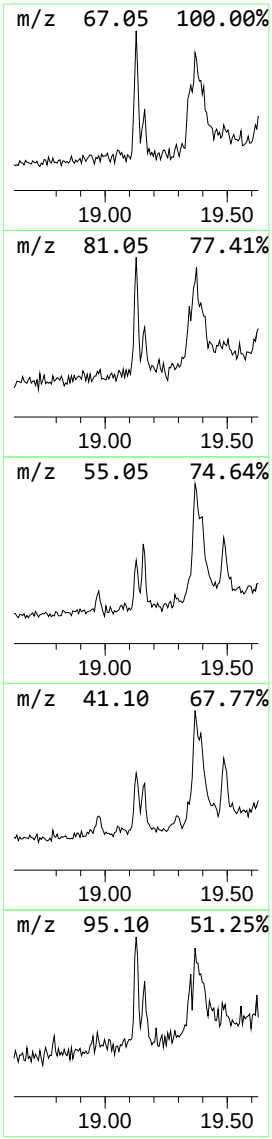
****

Peak Number 4 1-Pentadecyne Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.127	2.16 ng	36373	Phenanthrene-d10	17.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentadecyne	208	C15H28	000765-13-9	93
2	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	76
3	9-Octadecyne	250	C18H34	035365-59-4	68
4	1-Tetradecyne	194	C14H26	000765-10-6	68
5	1-Tridecyne	180	C13H24	026186-02-7	68





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one,...	4.381	37.5	ng	367038	1	7.963	196007	20.0
2-Pentanone, 4-...	5.016	20.8	ng	203704	1	7.963	196007	20.0
n-Hexadecanoic ...	18.215	3.5	ng	59689	4	17.345	336768	20.0
1-Pentadecyne	19.127	2.2	ng	36373	4	17.345	336768	20.0