LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080522\
Data File : BM036140.D
Acq On : 06 Aug 2022 03:56
Operator : CG/JU
Sample : N3961-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-172

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-BM080122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036140.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.957	312	318	329	rVB	229857	331454	2.46%	0.361%
2	5.445	394	401	415	rBV	5128188	7391571	54.83%	8.045%
3	7.069	670	677	689	rBV	4799061	7500202	55.64%	8.163%
4	7.857	803	811	818	rBV	1158955	1858151	13.78%	2.022%
5	9.028	1002	1010	1024	rBV	3007360	4865906	36.10%	5.296%
6	10.222	1207	1213	1223	rVB	82163	142380	1.06%	0.155%
7	10.657	1280	1287	1294	rBV	1535988	2560814	19.00%	2.787%
8	12.339	1566	1573	1588	rBV2	69755	266546	1.98%	0.290%
9	12.533	1600	1606	1618	rVB	151001	248578	1.84%	0.271%
10	12.657	1621	1627	1634	rBV	78426	141953	1.05%	0.154%
11	13.121	1695	1706	1718	rBV	7223729	10755698	79.79%	11.706%
12	14.145	1868	1880	1887	rBV7	65875	161258	1.20%	0.176%
13	14.221	1887	1893	1901	rVB	77002	136519	1.01%	0.149%
14	14.498	1933	1940	1946	rBV	2145993	3160173	23.44%	3.439%
15	15.986	2187	2193	2199	rBV	5459866	7815439	57.98%	8.506%
16	16.198	2225	2229	2239	rBV	135155	256322	1.90%	0.279%
17	16.645	2301	2305	2310	rBV4	92701	144440	1.07%	0.157%
18	17.145	2385	2390	2397	rBV2	200694	345599	2.56%	0.376%
19	17.239	2397	2406	2410	rVV	2549420	3676742	27.28%	4.002%
20	17.280	2410	2413	2417	rVV	584384	726320	5.39%	0.790%
21	17.327	2417	2421	2425	rVV2	130776	199566	1.48%	0.217%
22	17.368	2425	2428	2434	rVV2	83162	138741	1.03%	0.151%
23	17.456	2440	2443	2452	rVB3	84042	136878	1.02%	0.149%
24	17.598	2463	2467	2470	rBV	158830	211578	1.57%	0.230%
25	17.909	2516	2520	2525	rVB	190250	236365	1.75%	0.257%
26	18.027	2533	2540	2545	rBV	123920	255347	1.89%	0.278%
27	18.080	2545	2549	2553	rBV	307471	437955	3.25%	0.477%
28	18.145	2555	2560	2569	rVB	1395401	1900189	14.10%	2.068%
29	18.433	2605	2609	2615	rBV3	136419	246803	1.83%	0.269%
30	19.086	2717	2720	2723	rVB2	223478	236875	1.76%	0.258%
31	19.297	2751	2756	2758	rBV	460722	620184	4.60%	0.675%
32	19.321	2758	2760	2769	rVB3	212446	346683	2.57%	0.377%
33	19.415	2773	2776	2780	rBV	214465	264723	1.96%	0.288%
34	19.656	2813	2817	2826	rVB	412818	643903	4.78%	0.701%
35	19.862	2847	2852	2857	rBV	11071145	13479735	100.00%	14.671%
36	20.144	2897	2900	2903	rBV2	208665	251935	1.87%	0.274%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080522\
Data File : BM036140.D
Acq On : 06 Aug 2022 03:56
Operator : CG/JU
Sample : N3961-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-172

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-BM080122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.350	2932	2935	2940	rVB4	143002	174708	1.30%	0.190%
38	20.844	3016	3019	3022	rBV	262757	279388	2.07%	0.304%
39	20.886	3022	3026	3034	rVB	1518259	1711902	12.70%	1.863%
40	21.127	3063	3067	3074	rVB2	1338196	1645461	12.21%	1.791%
41	21.303	3094	3097	3100	rBV	433082	477869	3.55%	0.520%
42	21.415	3111	3116	3120	rBV	3042084	4030066	29.90%	4.386%
43	23.050	3390	3394	3399	rBV2	1149990	1934537	14.35%	2.105%
44	23.109	3400	3404	3412	rVB2	1054947	1822493	13.52%	1.984%
45	23.780	3512	3518	3525	rVB2	1837267	3582270	26.58%	3.899%
46	24.380	3614	3620	3629	rVB	1969631	4129495	30.63%	4.494%

Sum of corrected areas: 91881714

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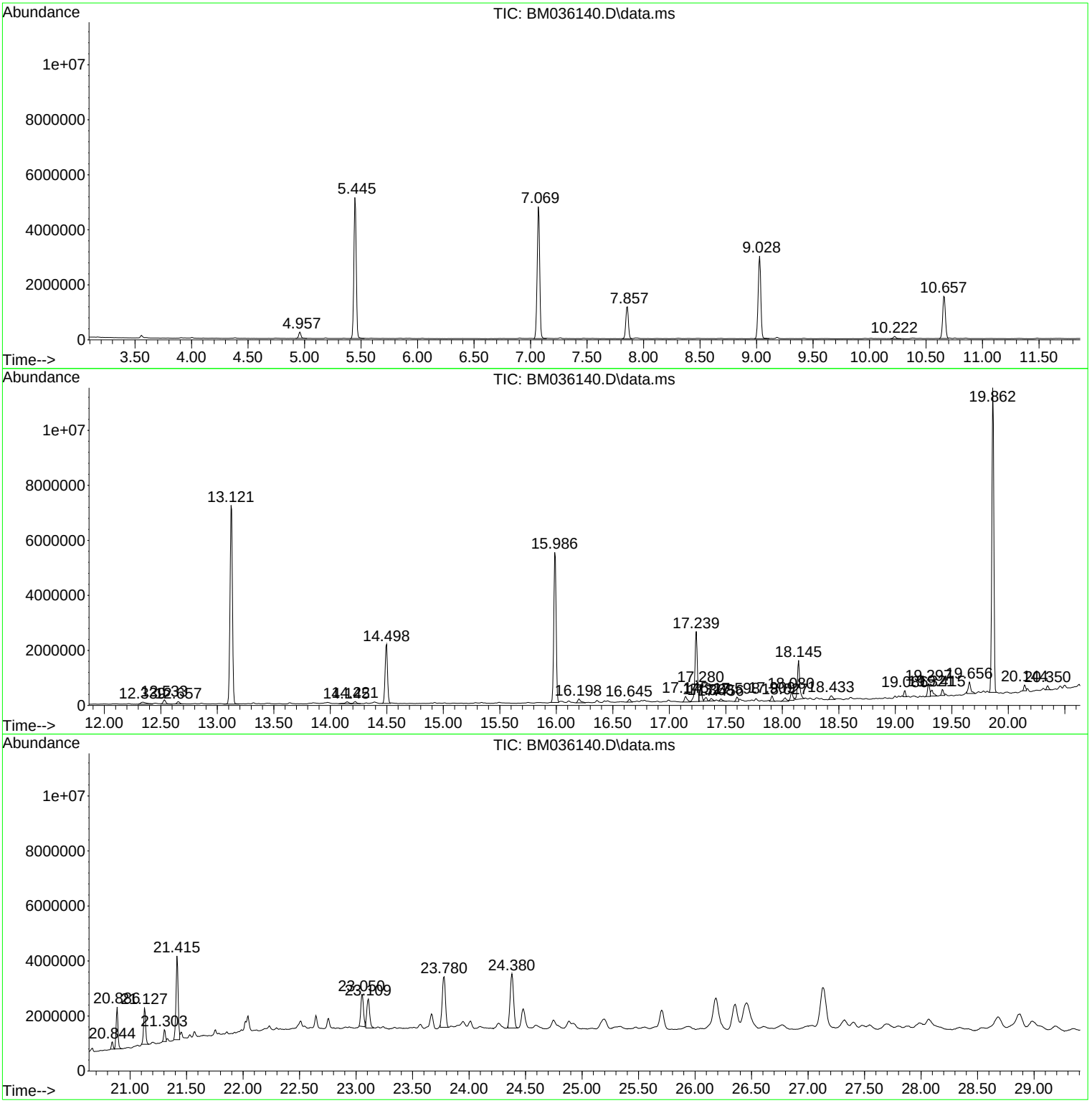
Instrument :
BNA_M
ClientSampleId :
RVE-172

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.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_M\Data\BM080522\
Data File : BM036140.D
Acq On : 06 Aug 2022 03:56
Operator : CG/JU
Sample : N3961-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-172

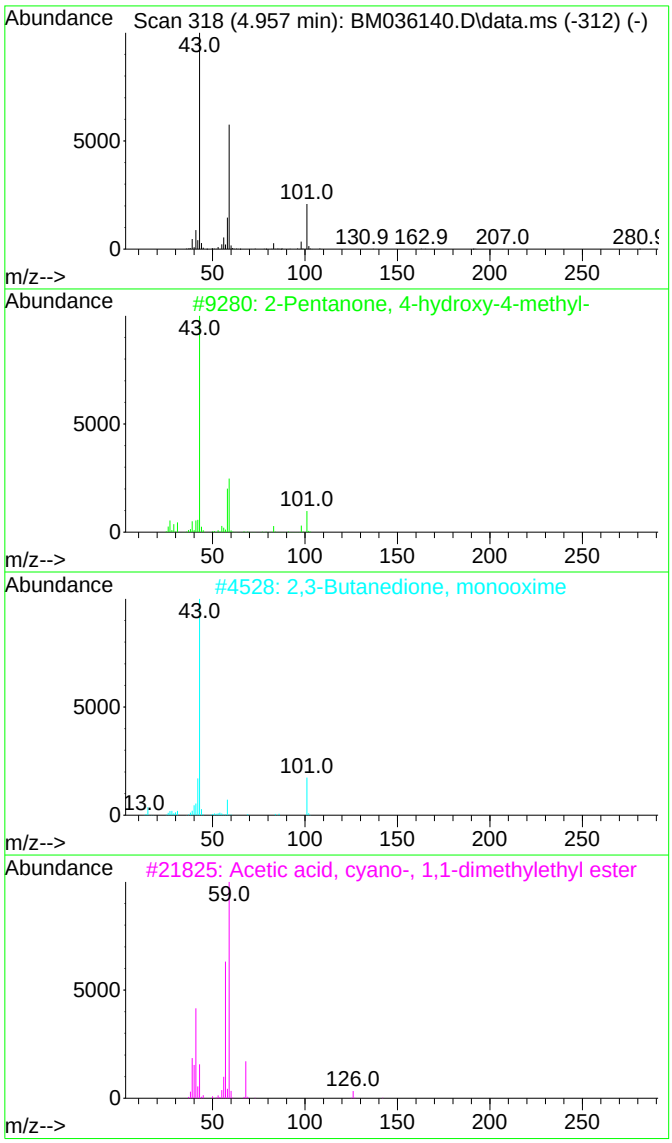
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

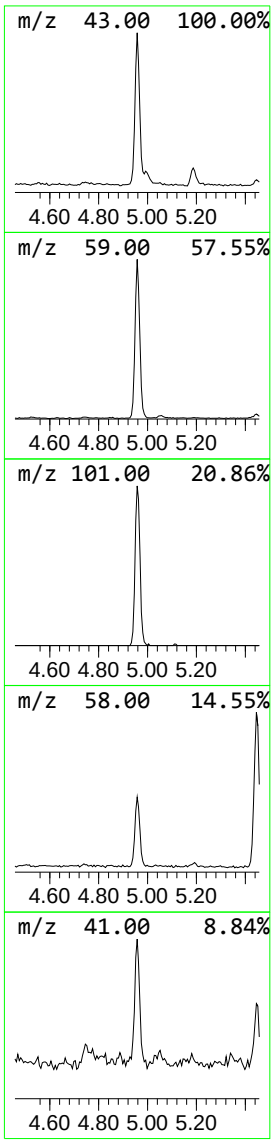
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.957	3.57 ng	331454	1,4-Dichlorobenzene-d4	7.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Data File : BM036140.D
Acq On : 06 Aug 2022 03:56
Operator : CG/JU
Sample : N3961-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-172

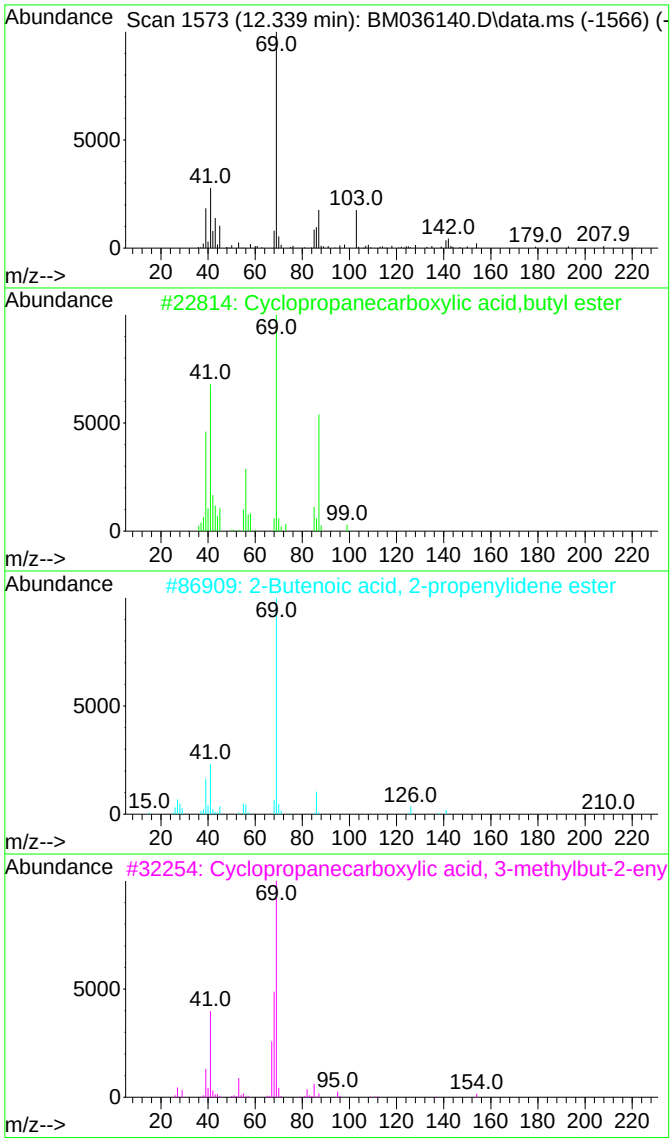
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

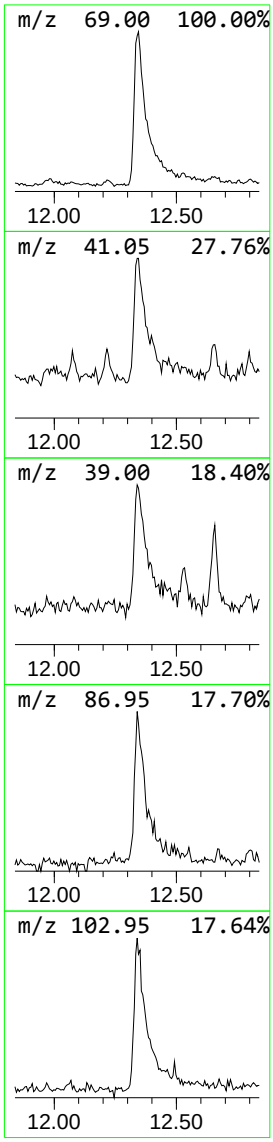
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclopropanecarboxylic acid... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.339	2.08 ng	266546	Naphthalene-d8	10.657

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropanecarboxylic acid,buty...	142	C8H14O2	054947-39-6	59
2	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	53
3	Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	47
4	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	45
5	Cyclopropanecarboxylic acid, pen...	150	C9H10O2	1010299-37-5	37





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Data File : BM036140.D
Acq On : 06 Aug 2022 03:56
Operator : CG/JU
Sample : N3961-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-172

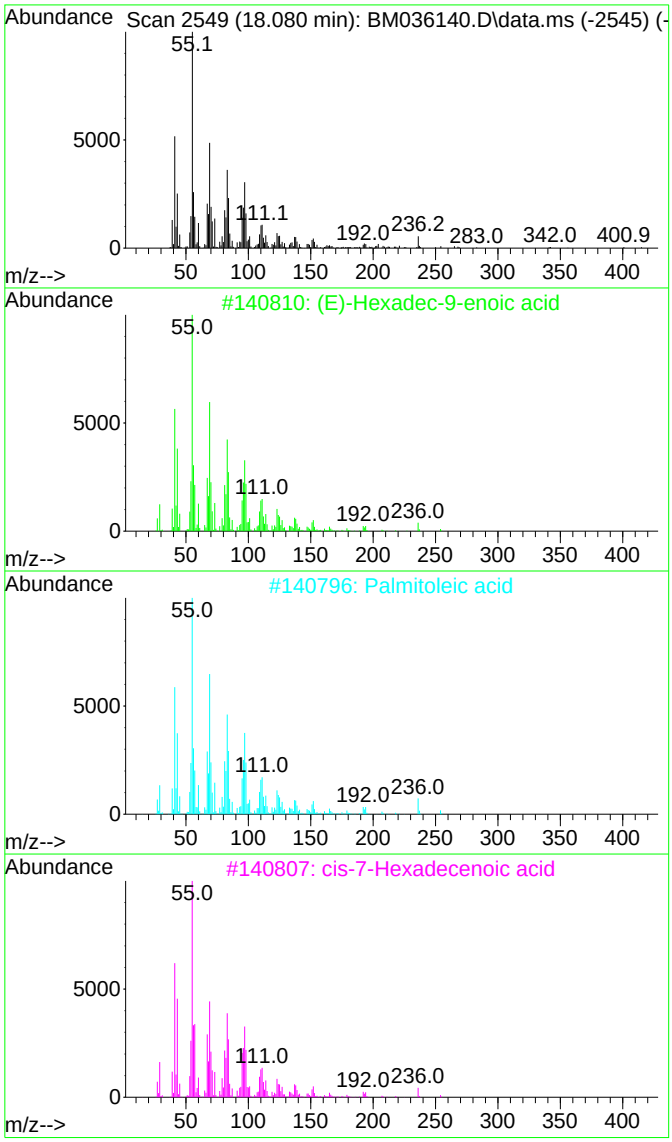
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

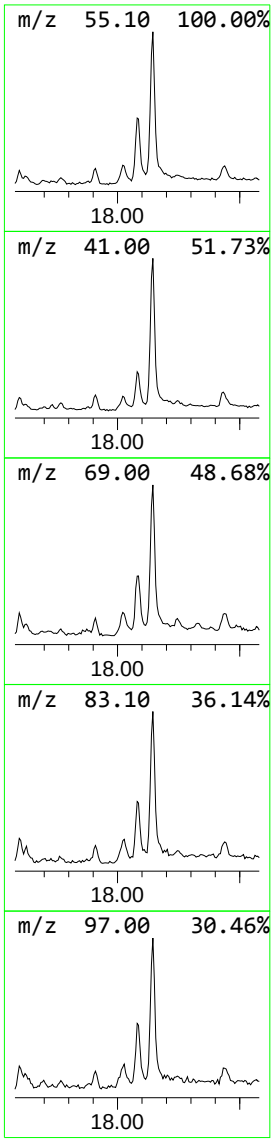
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (E)-Hexadec-9-enoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.080	2.38 ng	437955	Phenanthrene-d10	17.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	99
2	Palmitoleic acid	254	C16H30O2	000373-49-9	96
3	cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	96
4	cis-10-Heptadecenoic acid	268	C17H32O2	029743-97-3	95
5	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	94





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Sample : N3961-05
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

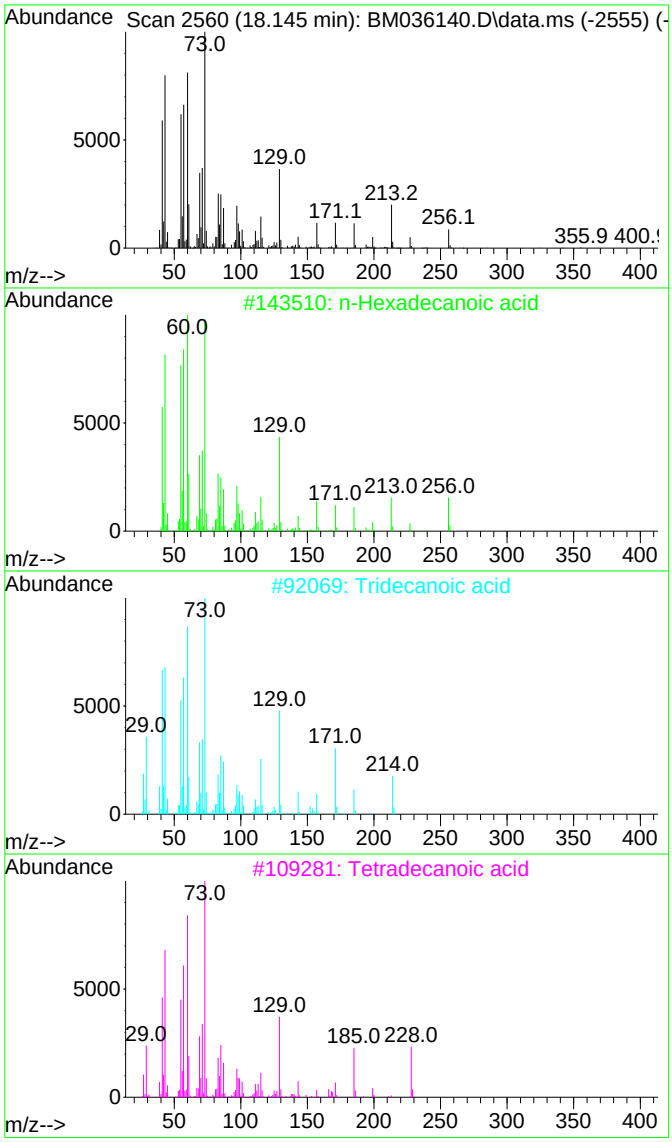
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

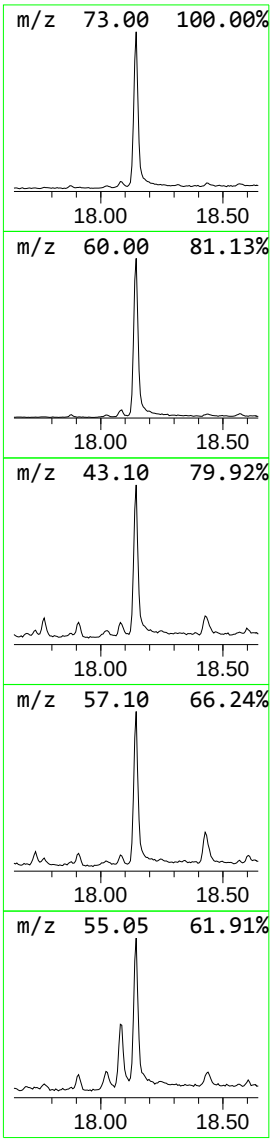
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.145	10.34 ng	1900190	Phenanthrene-d10	17.239

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	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	Octadecanoic acid	284	C18H36O2	000057-11-4	76





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Sample : N3961-05
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-172

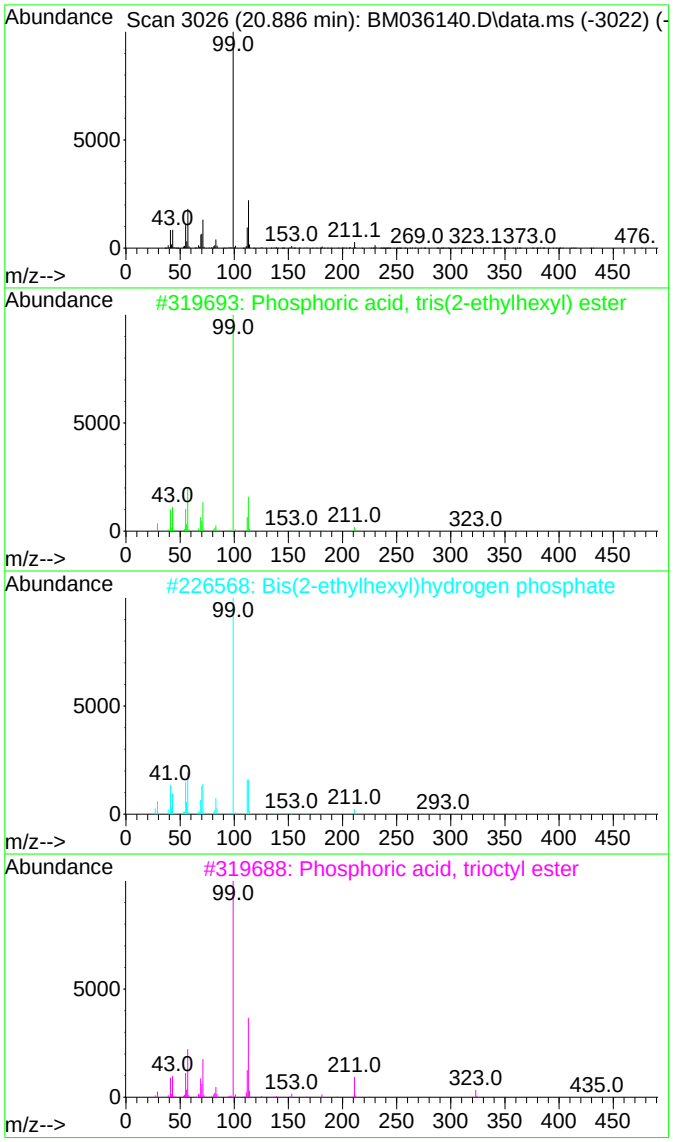
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

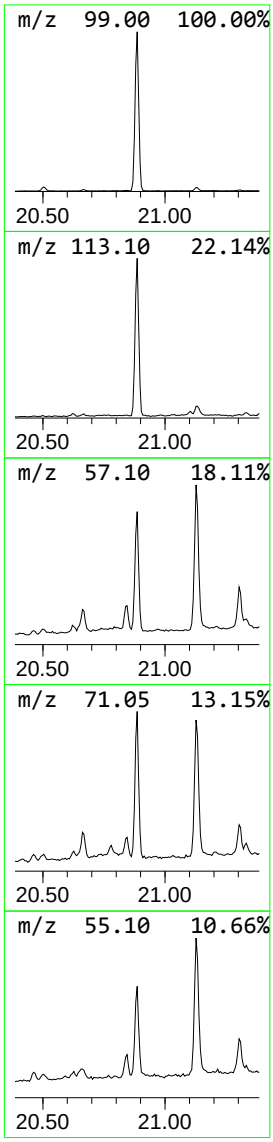
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Phosphoric acid, tris(2-eth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.886	8.50 ng	1711900	Chrysene-d12	21.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosphoric acid, tris(2-ethylhex...	434	C24H51O4P	000078-42-2	86
2	Bis(2-ethylhexyl)hydrogen phosphate	322	C16H35O4P	000298-07-7	56
3	Phosphoric acid, trioctyl ester	434	C24H51O4P	001806-54-8	52
4	Triisobutyl phosphate	266	C12H27O4P	000126-71-6	45
5	2,4,4-Trimethyl-1-pentyl methylp...	210	C9H20FO2P	333416-06-1	42





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-172

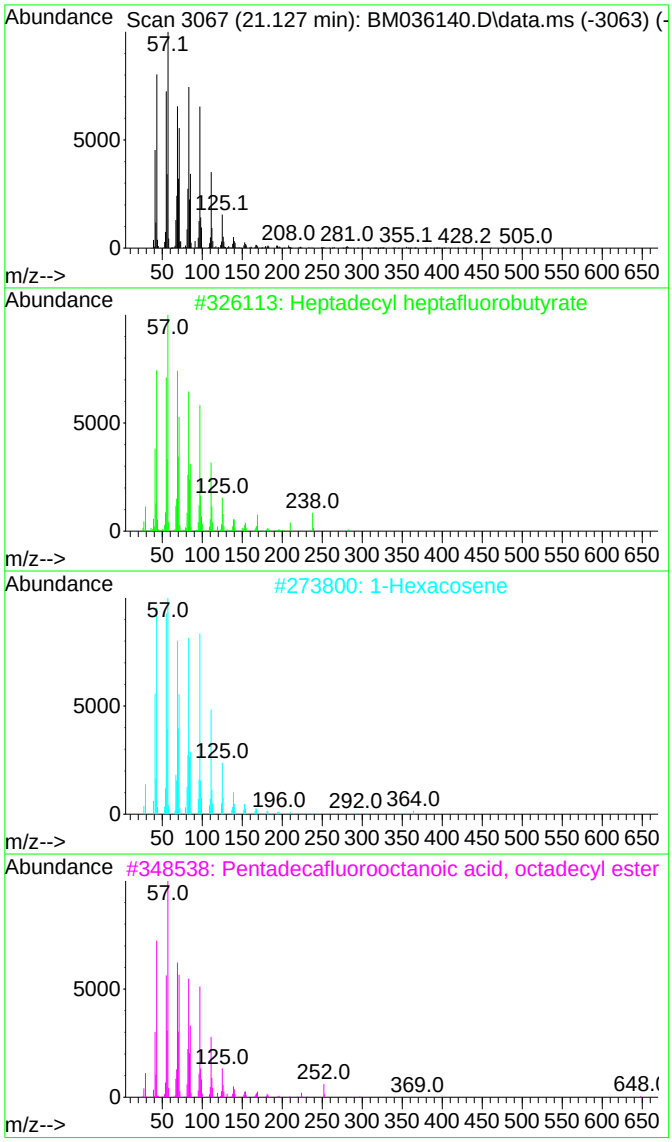
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

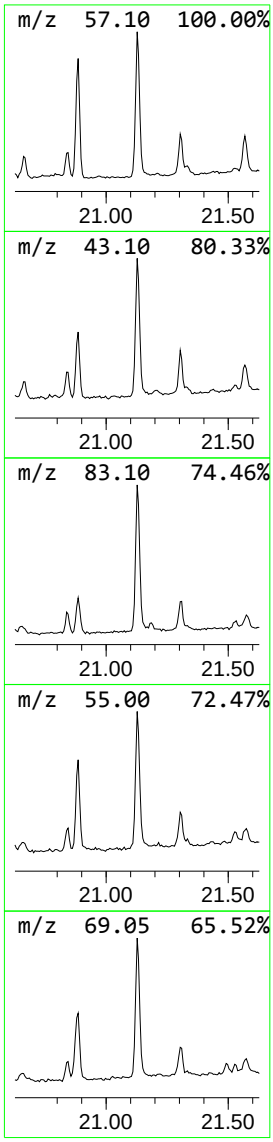
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	8.17 ng	1645460	Chrysene-d12	21.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	1-Hexacosene	364	C26H52	018835-33-1	94
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	17-Pentatriacontene	491	C35H70	006971-40-0	93





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

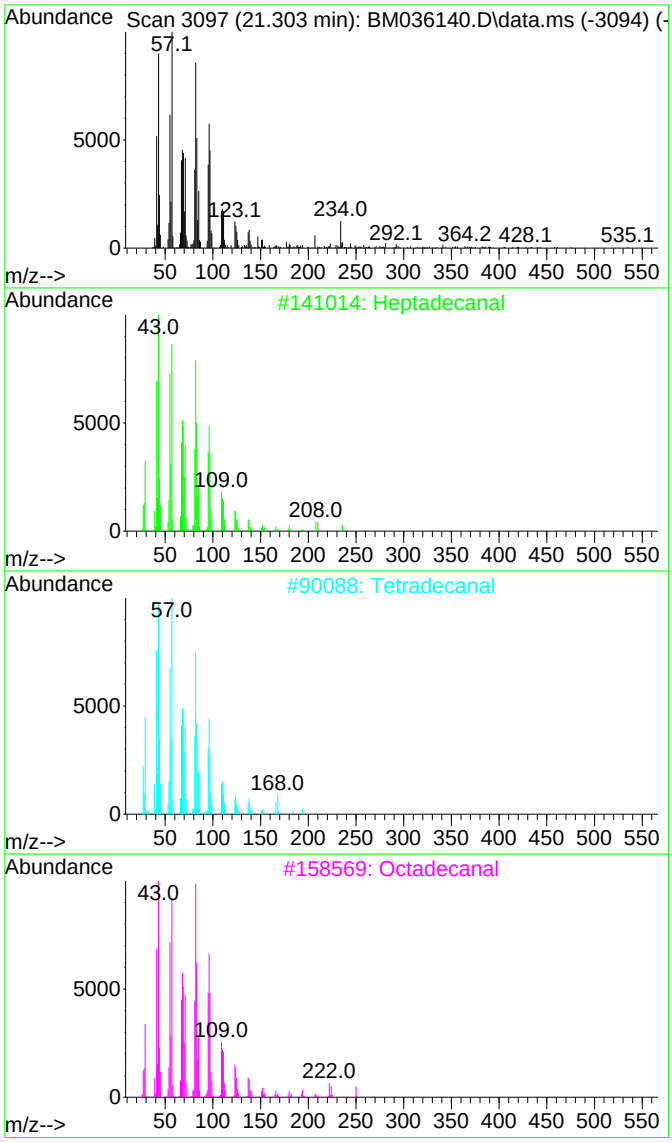
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

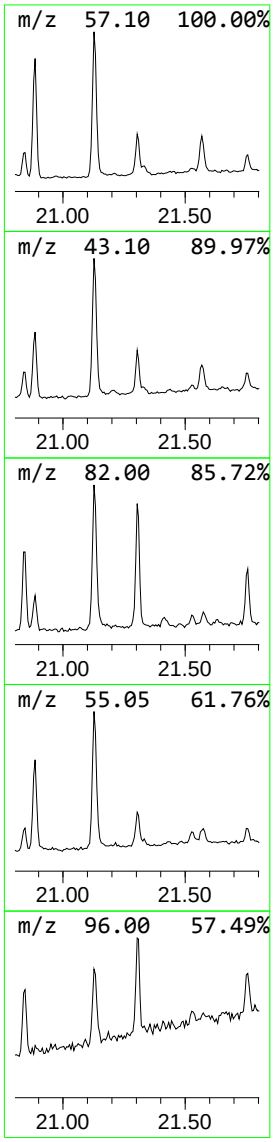
****

Peak Number 7 Heptadecanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.303	2.37 ng	477869	Chrysene-d12	21.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanal	254	C17H34O	1000376-70-0	95
2	Tetradecanal	212	C14H28O	000124-25-4	91
3	Octadecanal	268	C18H36O	000638-66-4	91
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
5	Eicosanal-	296	C20H40O	002400-66-0	90





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Data File : BM036140.D
Acq On : 06 Aug 2022 03:56
Operator : CG/JU
Sample : N3961-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-172

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

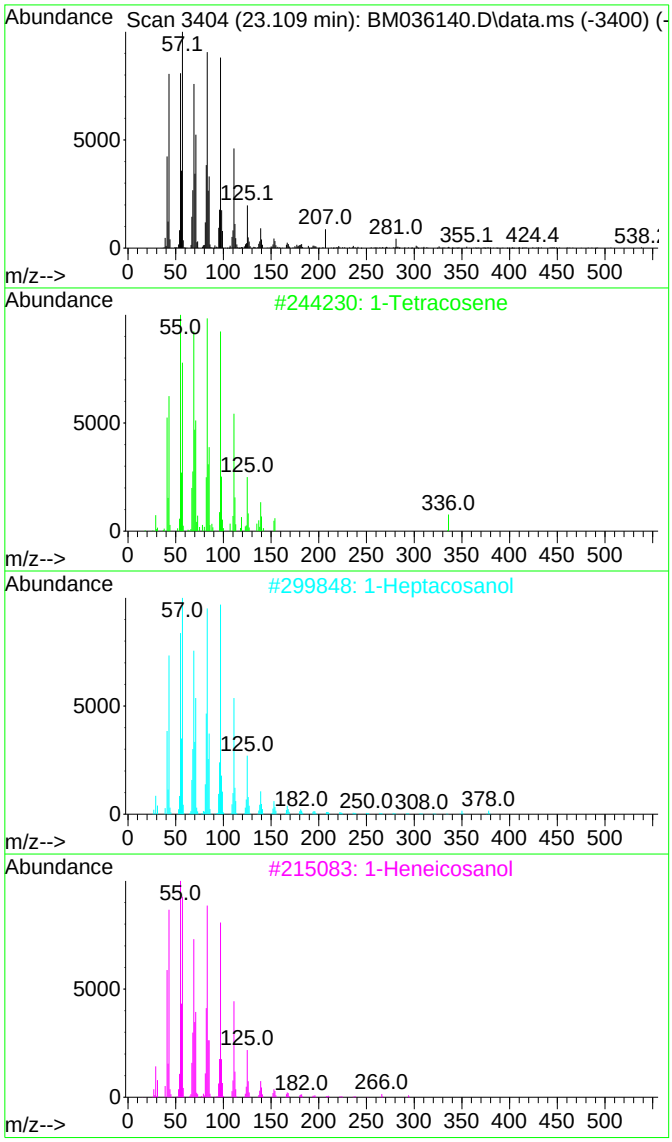
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

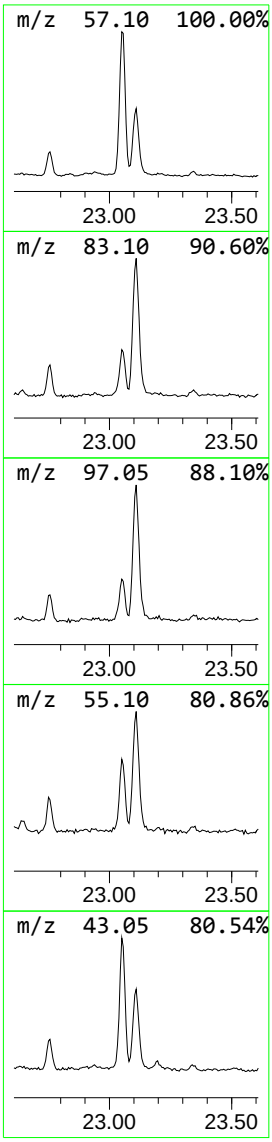
****

Peak Number 8 1-Tetracosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.109	10.18 ng	1822490	Perylene-d12	23.780

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	99
2	1-Heptacosanol	396	C27H56O	002004-39-9	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	1-Hexacosene	364	C26H52	018835-33-1	94
5	Heptacos-1-ene	378	C27H54	015306-27-1	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080522\
Data File : BM036140.D
Acq On : 06 Aug 2022 03:56
Operator : CG/JU
Sample : N3961-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-172

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

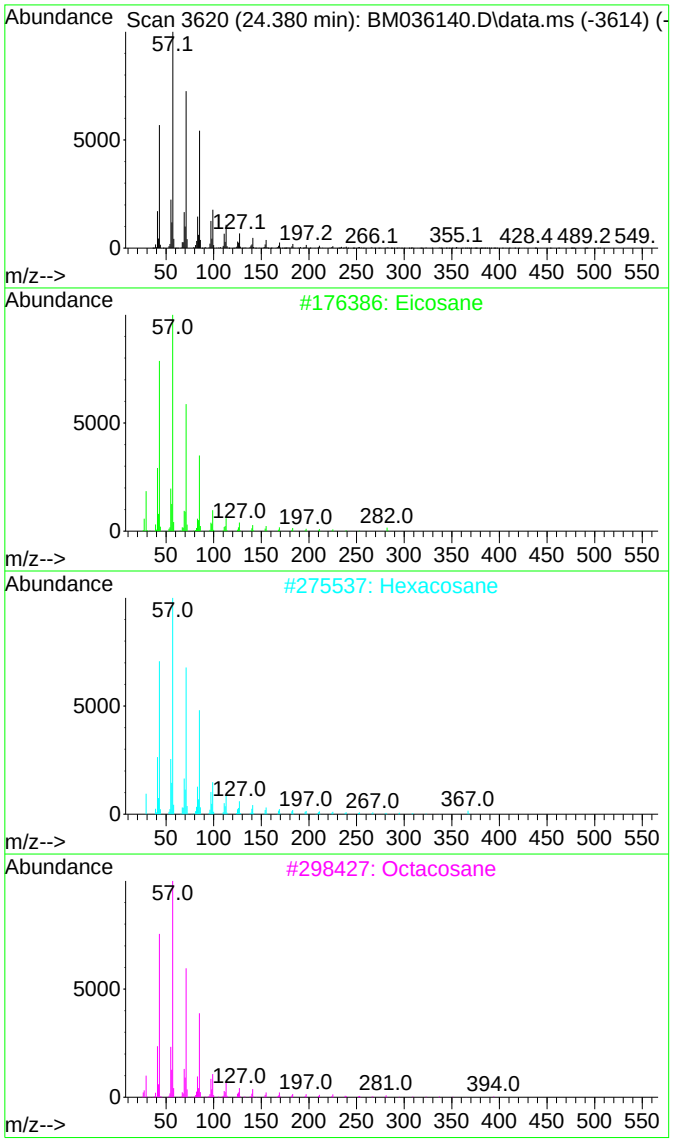
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

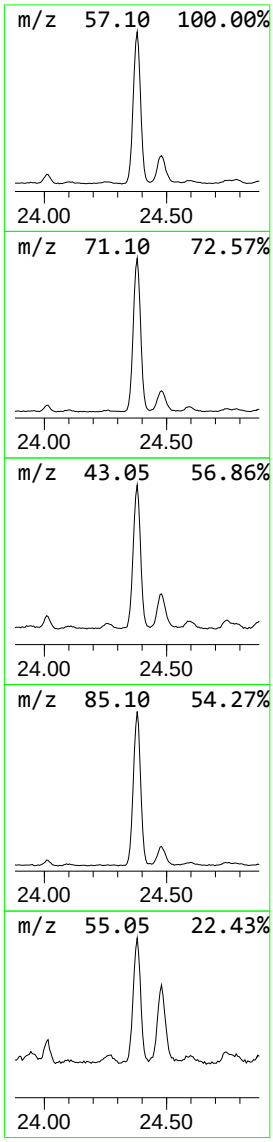
****

Peak Number 9 Eicosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.380	23.06 ng	4129500	Perylene-d12	23.780

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Hexacosane	366	C26H54	000630-01-3	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
5	Heneicosane	296	C21H44	000629-94-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080522\
Data File : BM036140.D
Acq On : 06 Aug 2022 03:56
Operator : CG/JU
Sample : N3961-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-172

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.957	3.6	ng	331454	1	7.857	1858150	20.0
Cyclopropanecar...	12.339	2.1	ng	266546	2	10.657	2560810	20.0
(E)-Hexadec-9-e...	18.080	2.4	ng	437955	4	17.239	3676740	20.0
n-Hexadecanoic ...	18.145	10.3	ng	1900190	4	17.239	3676740	20.0
Phosphoric acid...	20.886	8.5	ng	1711900	5	21.415	4030070	20.0
Heptadecyl hept...	21.127	8.2	ng	1645460	5	21.415	4030070	20.0
Heptadecanal	21.303	2.4	ng	477869	5	21.415	4030070	20.0
1-Tetracosene	23.109	10.2	ng	1822490	6	23.780	3582270	20.0
Eicosane	24.380	23.1	ng	4129500	6	23.780	3582270	20.0