LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033123\
Data File : BM039267.D
Acq On : 31 Mar 2023 23:41
Operator : CG/JU
Sample : 02104-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-37-SB01

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-BM032923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039267.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.010	285	293	304	rBV	1410823	1920139	27.58%	3.523%
2	5.475	366	372	390	rBV	3143459	4532793	65.10%	8.316%
3	7.087	634	646	660	rBV	2888380	4516356	64.86%	8.286%
4	7.916	778	787	794	rBV	803646	1261280	18.11%	2.314%
5	8.134	819	824	831	rBV	210667	312286	4.48%	0.573%
6	9.087	979	986	992	rBV	1767468	2836416	40.74%	5.204%
7	9.145	992	996	1002	rVB	69691	106946	1.54%	0.196%
8	10.728	1253	1265	1271	rBV	958949	1722784	24.74%	3.161%
9	10.781	1271	1274	1280	rVB	60707	90954	1.31%	0.167%
10	12.145	1497	1506	1511	rBV	91978	136505	1.96%	0.250%
11	12.386	1541	1547	1555	rVB2	43114	78409	1.13%	0.144%
12	13.186	1676	1683	1694	rBV	4012605	5641664	81.02%	10.350%
13	13.386	1712	1717	1723	rVB2	109834	176299	2.53%	0.323%
14	13.886	1797	1802	1807	rBV	36089	71636	1.03%	0.131%
15	14.039	1821	1828	1832	rBV2	43789	72877	1.05%	0.134%
16	14.416	1884	1892	1895	rBV6	29743	79983	1.15%	0.147%
17	14.457	1895	1899	1906	rVB	114650	161766	2.32%	0.297%
18	14.563	1907	1917	1923	rBV	1249893	1852823	26.61%	3.399%
19	14.627	1923	1928	1936	rVB	175212	273865	3.93%	0.502%
20	14.963	1980	1985	1991	rBV2	99077	149278	2.14%	0.274%
21	15.404	2056	2060	2065	rVB	89397	111268	1.60%	0.204%
22	15.610	2090	2095	2100	rBV	154283	230253	3.31%	0.422%
23	15.921	2141	2148	2153	rBV	346565	504265	7.24%	0.925%
24	16.051	2164	2170	2180	rBV	2788298	3995118	57.38%	7.330%
25	16.268	2203	2207	2209	rBV	101388	133384	1.92%	0.245%
26	16.557	2252	2256	2260	rBV	129567	178532	2.56%	0.328%
27	16.910	2313	2316	2321	rVB	83298	107947	1.55%	0.198%
28	17.063	2339	2342	2346	rVB	80891	87608	1.26%	0.161%
29	17.310	2379	2384	2388	rBV	1496960	2070419	29.73%	3.798%
30	17.351	2388	2391	2398	rVV	961777	1307172	18.77%	2.398%
31	17.445	2402	2407	2412	rVV	226977	318369	4.57%	0.584%
32	17.721	2450	2454	2460	rVB	99440	140287	2.01%	0.257%
33	17.804	2465	2468	2471	rVB	70744	73136	1.05%	0.134%
34	18.210	2530	2537	2540	rBV2	459398	798235	11.46%	1.464%
35	18.386	2563	2567	2571	rBV3	139938	207375	2.98%	0.380%
36	18.498	2583	2586	2590	rBV2	87227	99377	1.43%	0.182%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033123\
Data File : BM039267.D
Acq On : 31 Mar 2023 23:41
Operator : CG/JU
Sample : 02104-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-37-SB01

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-BM032923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.633	2605	2609	2613	rBV2	189664	239633	3.44%	0.440%
38	19.368	2729	2734	2740	rBV	1260808	1627676	23.38%	2.986%
39	19.480	2751	2753	2759	rBV	129121	159866	2.30%	0.293%
40	19.704	2787	2791	2792	rBV2	251047	298629	4.29%	0.548%
41	19.733	2792	2796	2805	rVB	997912	1481801	21.28%	2.719%
42	19.933	2825	2830	2835	rBV	5761244	6962981	100.00%	12.774%
43	21.198	3042	3045	3054	rVB3	802777	1114044	16.00%	2.044%
44	21.403	3077	3080	3084	rVB	499691	536274	7.70%	0.984%
45	21.492	3089	3095	3099	rBV2	2083067	3407926	48.94%	6.252%
46	23.909	3501	3506	3512	rVB2	1205117	2320515	33.33%	4.257%

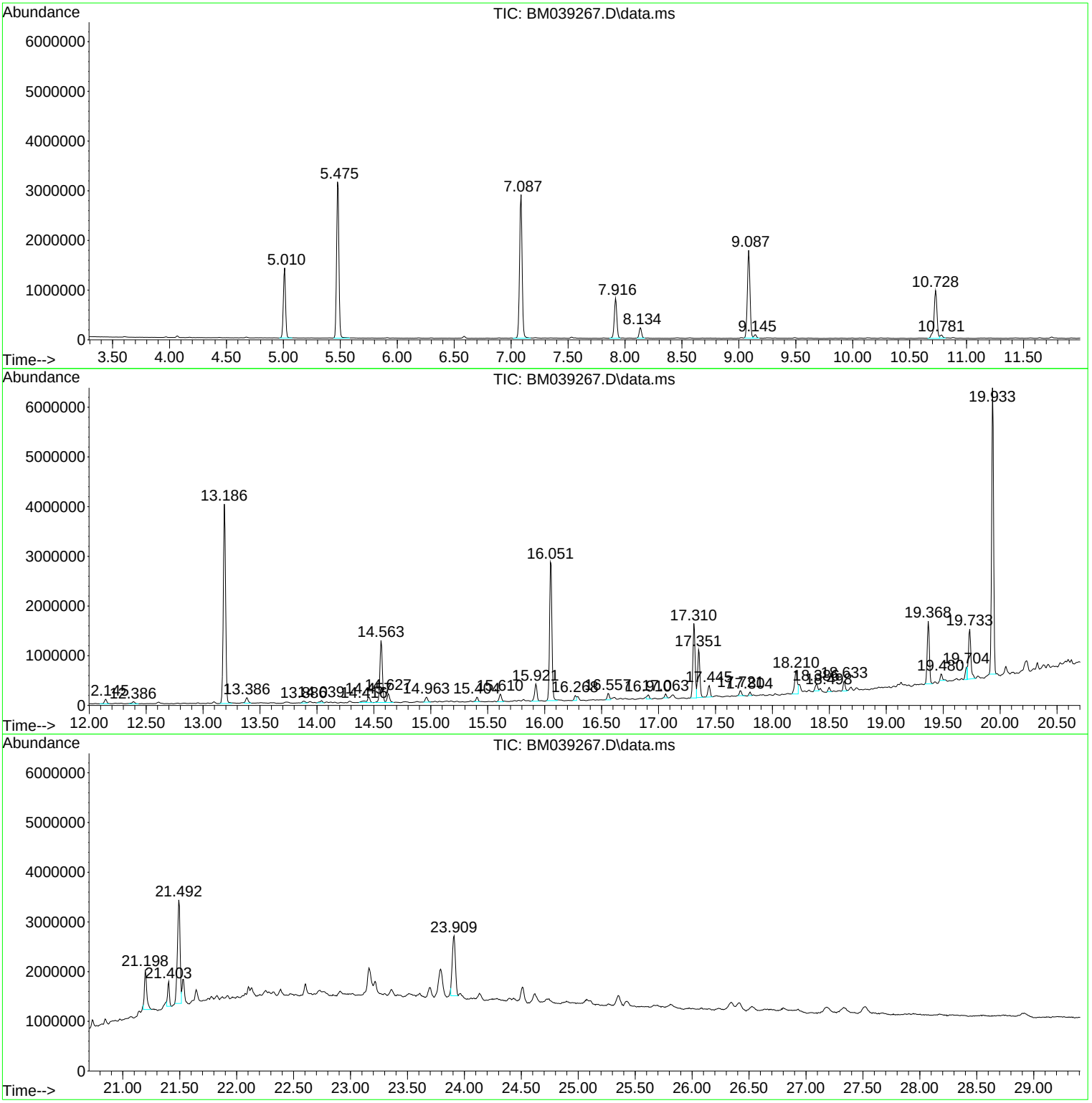
Sum of corrected areas: 54507149

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033123\
Data File : BM039267.D
Acq On : 31 Mar 2023 23:41
Operator : CG/JU
Sample : 02104-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-37-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.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\BM033123\
Data File : BM039267.D
Acq On : 31 Mar 2023 23:41
Operator : CG/JU
Sample : 02104-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-37-SB01

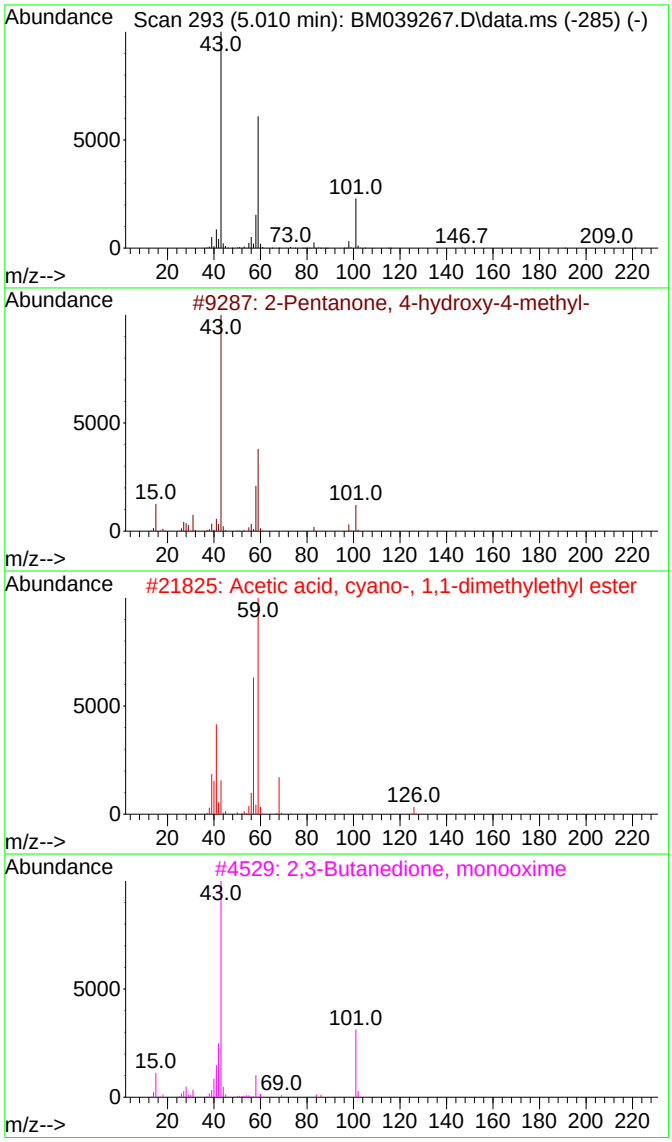
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

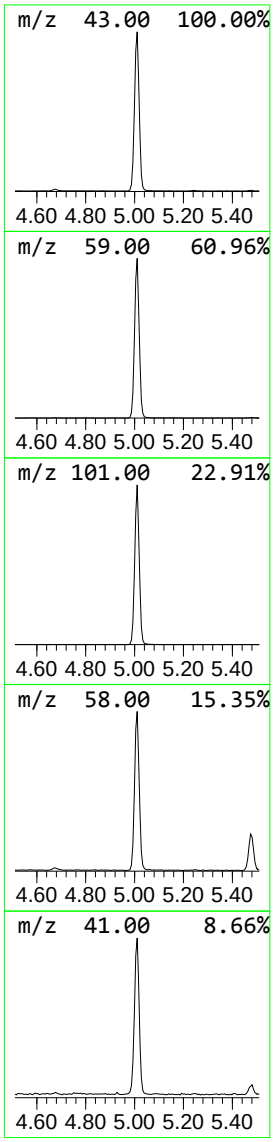
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.010	30.45 ng	1920140	1,4-Dichlorobenzene-d4	7.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033123\
Data File : BM039267.D
Acq On : 31 Mar 2023 23:41
Operator : CG/JU
Sample : 02104-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-37-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

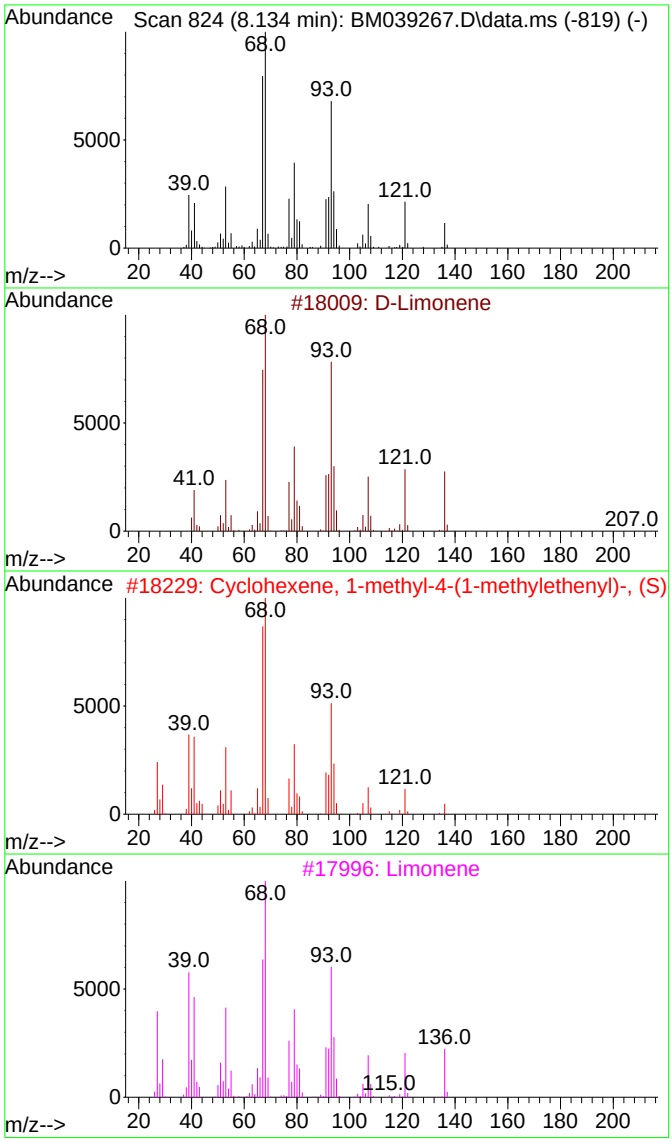
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

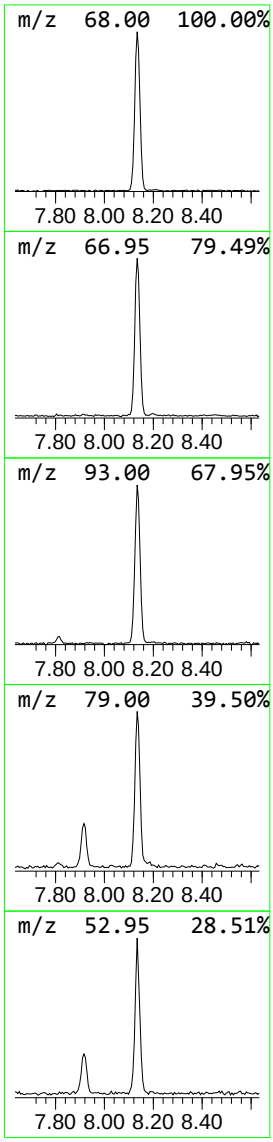
****

Peak Number 2 D-Limonene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.134	4.95 ng	312286	1,4-Dichlorobenzene-d4	7.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Limonene	136	C10H16	005989-27-5	98
2	Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	94
3	Limonene	136	C10H16	000138-86-3	91
4	Cyclohexene, 1-methyl-5-(1-methy...	136	C10H16	013898-73-2	86
5	Cyclohexanol, 1-methyl-4-(1-meth...	196	C12H20O2	010198-23-9	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033123\
Data File : BM039267.D
Acq On : 31 Mar 2023 23:41
Operator : CG/JU
Sample : 02104-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-37-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

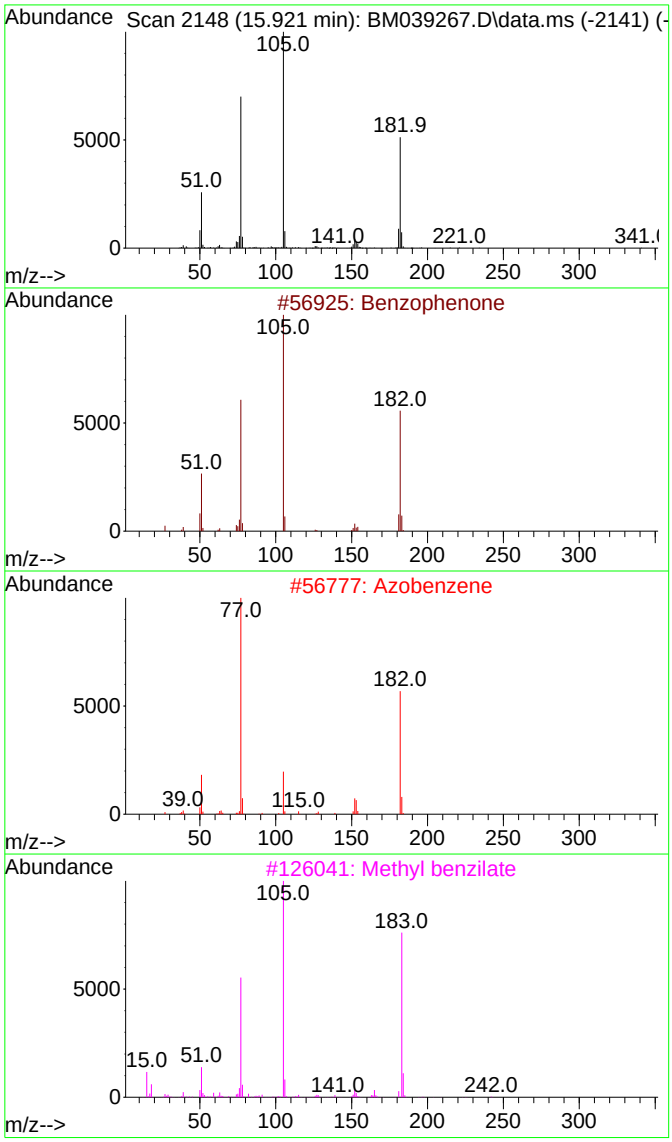
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

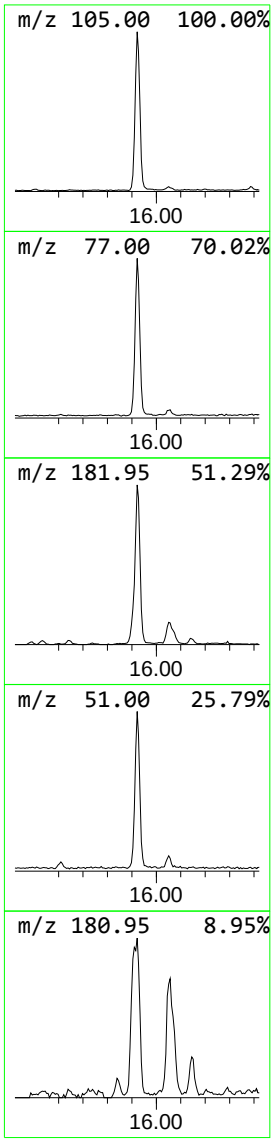
****

Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	5.44 ng	504265	Acenaphthene-d10	14.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	64
3	Methyl benzilate	242	C15H14O3	000076-89-1	47
4	Ethanone, 2-hydroxy-1-phenyl-	136	C8H8O2	000582-24-1	47
5	Vinyl benzoate	148	C9H8O2	000769-78-8	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033123\
Data File : BM039267.D
Acq On : 31 Mar 2023 23:41
Operator : CG/JU
Sample : 02104-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-37-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

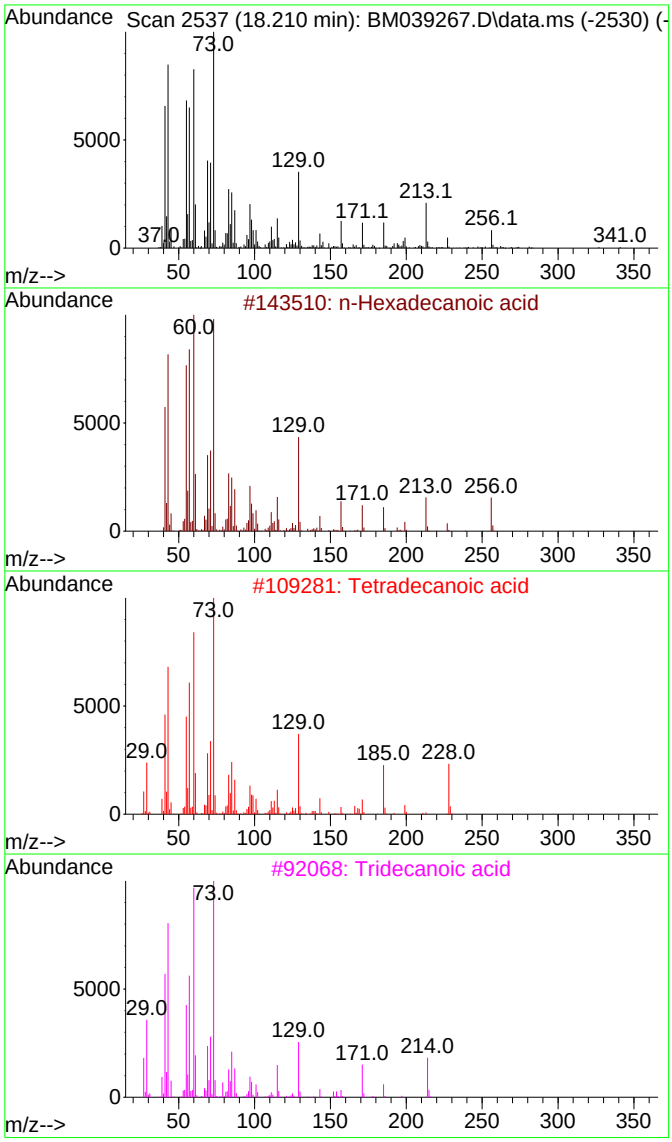
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

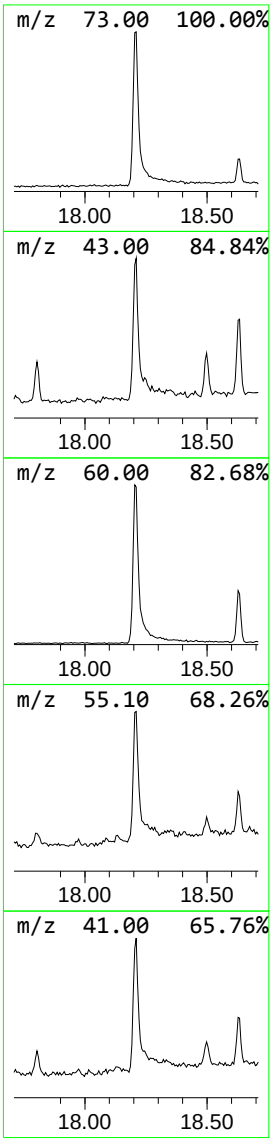
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.209	7.71 ng	798235	Phenanthrene-d10	17.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5	Tetradecane	198	C14H30	000629-59-4	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033123\
Data File : BM039267.D
Acq On : 31 Mar 2023 23:41
Operator : CG/JU
Sample : 02104-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-37-SB01

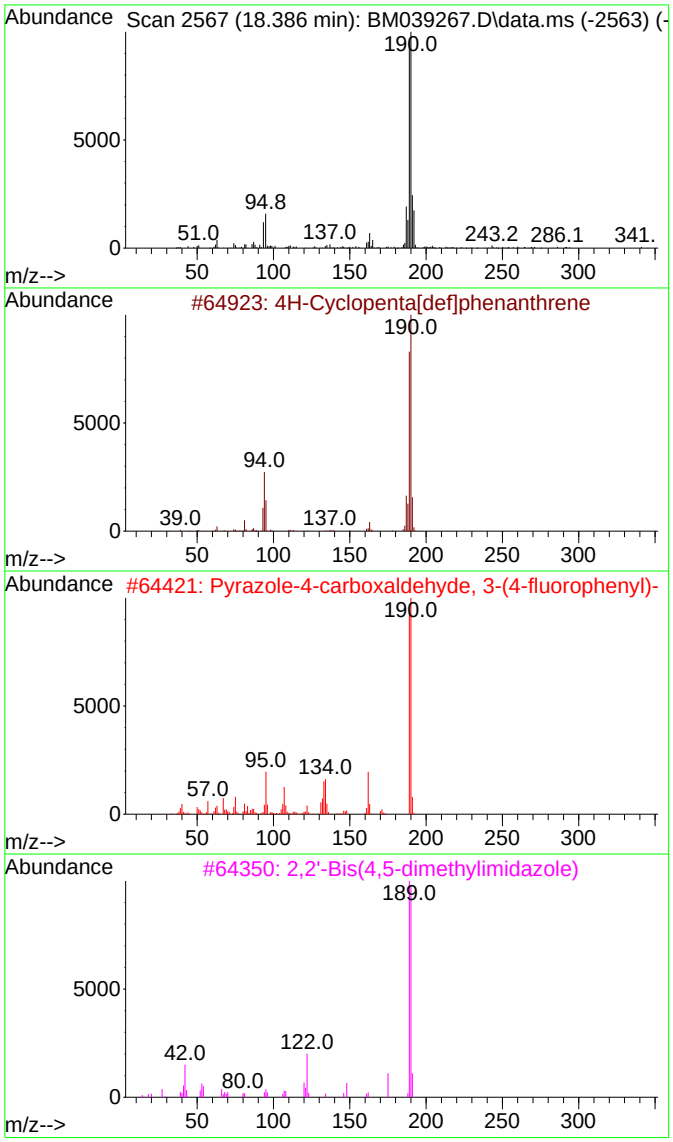
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

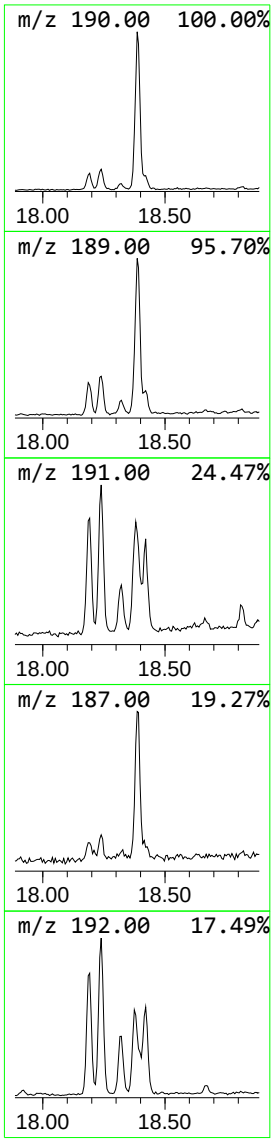
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.386	2.00 ng	207375	Phenanthrene-d10	17.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	90
2	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	42
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42
4	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	36
5	Benzo[1,2-b:4,3-b']dithiophene	190	C10H6S2	000210-80-0	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033123\
Data File : BM039267.D
Acq On : 31 Mar 2023 23:41
Operator : CG/JU
Sample : 02104-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-37-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

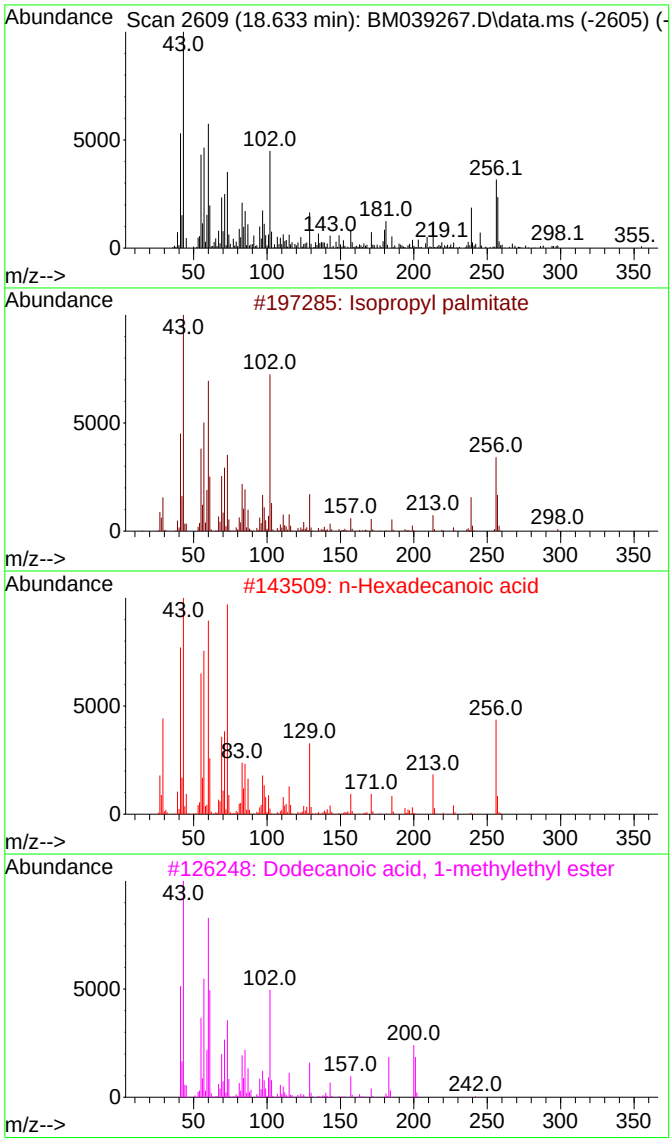
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

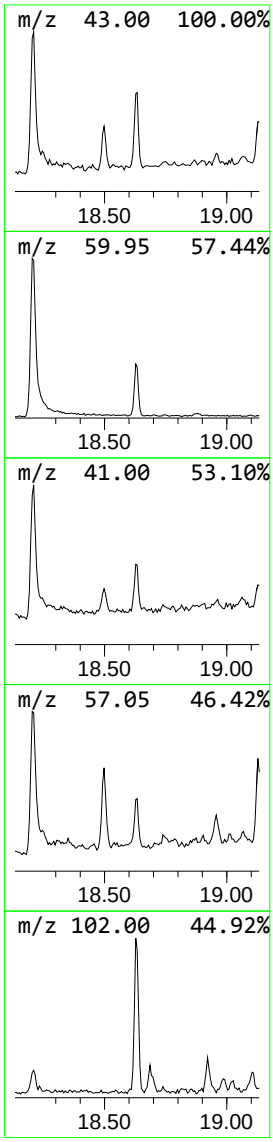
****

Peak Number 6 Isopropyl palmitate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.633	2.31 ng	239633	Phenanthrene-d10	17.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl palmitate	298	C19H38O2	000142-91-6	96
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
3	Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	43
4	8-Methylnonanoic acid, isopropyl...	214	C13H26O2	1000452-00-6	35
5	Nonadecanoic acid	298	C19H38O2	000646-30-0	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033123\
Data File : BM039267.D
Acq On : 31 Mar 2023 23:41
Operator : CG/JU
Sample : 02104-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-37-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

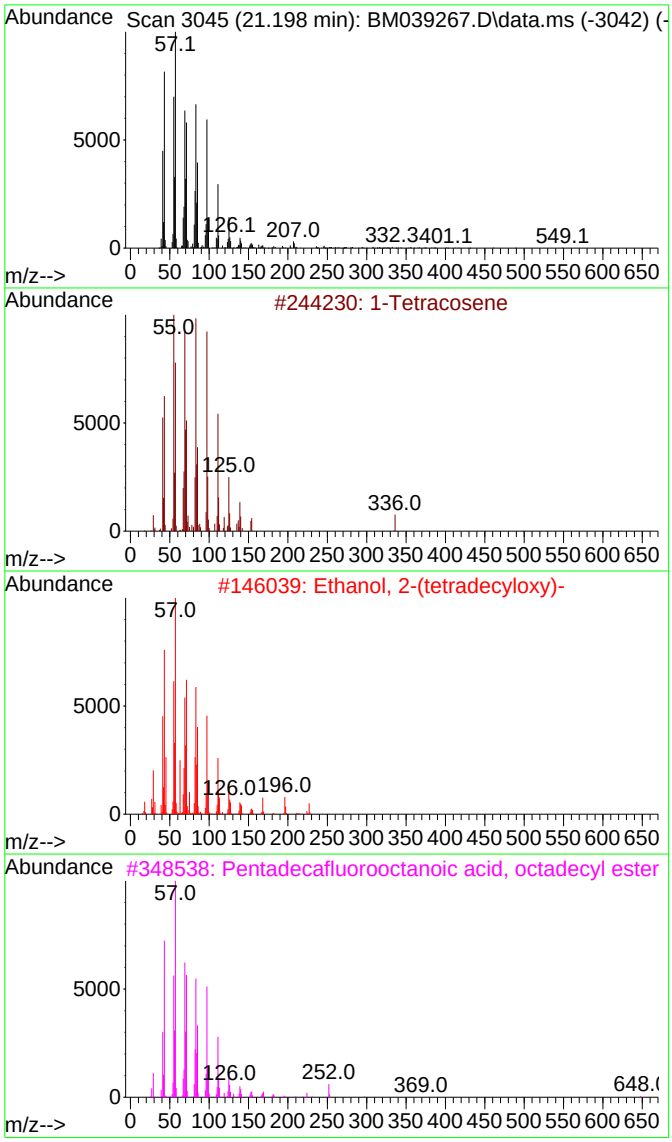
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

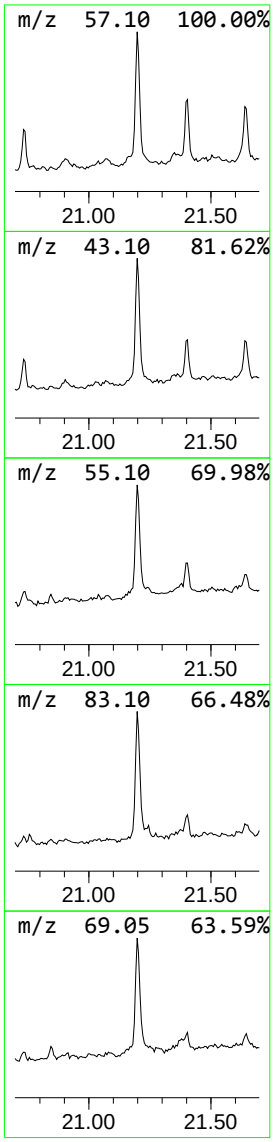
****

Peak Number 7 1-Tetracosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.198	6.54 ng	1114040	Chrysene-d12	21.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	97
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	96
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033123\
Data File : BM039267.D
Acq On : 31 Mar 2023 23:41
Operator : CG/JU
Sample : 02104-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-37-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.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-...	5.010	30.4	ng	1920140	1	7.916	1261280	20.0
D-Limonene	8.134	5.0	ng	312286	1	7.916	1261280	20.0
Benzophenone	15.921	5.4	ng	504265	3	14.563	1852820	20.0
n-Hexadecanoic ...	18.209	7.7	ng	798235	4	17.310	2070420	20.0
4H-Cyclopenta[d...	18.386	2.0	ng	207375	4	17.310	2070420	20.0
Isopropyl palmi...	18.633	2.3	ng	239633	4	17.310	2070420	20.0
1-Tetracosene	21.198	6.5	ng	1114040	5	21.492	3407930	20.0