LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062023\
Data File : BG057779.D
Acq On : 20 Jun 2023 16:54
Operator : CG/JU
Sample : 03255-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSIT-SB-24

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_G\Methods\8270-BG061923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057779.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.039	325	332	344	rVB	81951	131312	2.90%	0.741%
2	5.503	404	411	419	rBV	623437	1012244	22.35%	5.710%
3	7.090	673	681	689	rBV	642870	1085755	23.98%	6.125%
4	7.930	815	824	835	rBV	174372	304098	6.72%	1.716%
5	9.087	1014	1021	1029	rBV	387407	663192	14.64%	3.741%
6	10.733	1290	1301	1306	rBV	235486	457870	10.11%	2.583%
7	13.189	1710	1719	1727	rVB	907633	1440535	31.81%	8.126%
8	14.563	1944	1953	1959	rBV	356685	559956	12.37%	3.159%
9	14.957	2015	2020	2026	rVB	31689	51664	1.14%	0.291%
10	15.915	2177	2183	2188	rVB2	59138	94826	2.09%	0.535%
11	16.044	2199	2205	2214	rVB	673057	1062765	23.47%	5.995%
12	17.307	2414	2420	2424	rBV	401189	625200	13.81%	3.527%
13	17.348	2424	2427	2432	rVB	191933	257079	5.68%	1.450%
14	17.437	2438	2442	2447	rBV	48355	69556	1.54%	0.392%
15	18.136	2557	2561	2565	rBV2	45442	59551	1.32%	0.336%
16	18.194	2565	2571	2575	rBV3	280898	413753	9.14%	2.334%
17	18.377	2597	2602	2606	rBV2	49984	85139	1.88%	0.480%
18	19.358	2764	2769	2776	rBV	495392	681300	15.04%	3.843%
19	19.469	2784	2788	2792	rBV2	134504	174521	3.85%	0.985%
20	19.722	2822	2831	2839	rVB	406578	699758	15.45%	3.948%
21	19.922	2860	2865	2870	rBV	1303177	1638117	36.17%	9.241%
22	21.214	3082	3085	3093	rVB3	162136	265478	5.86%	1.498%
23	21.461	3121	3127	3133	rVV	3285667	4528465	100.00%	25.546%
24	21.555	3136	3143	3148	rVV2	427211	1036376	22.89%	5.846%
25	21.608	3149	3152	3160	rVB	208443	327948	7.24%	1.850%

Sum of corrected areas: 17726458

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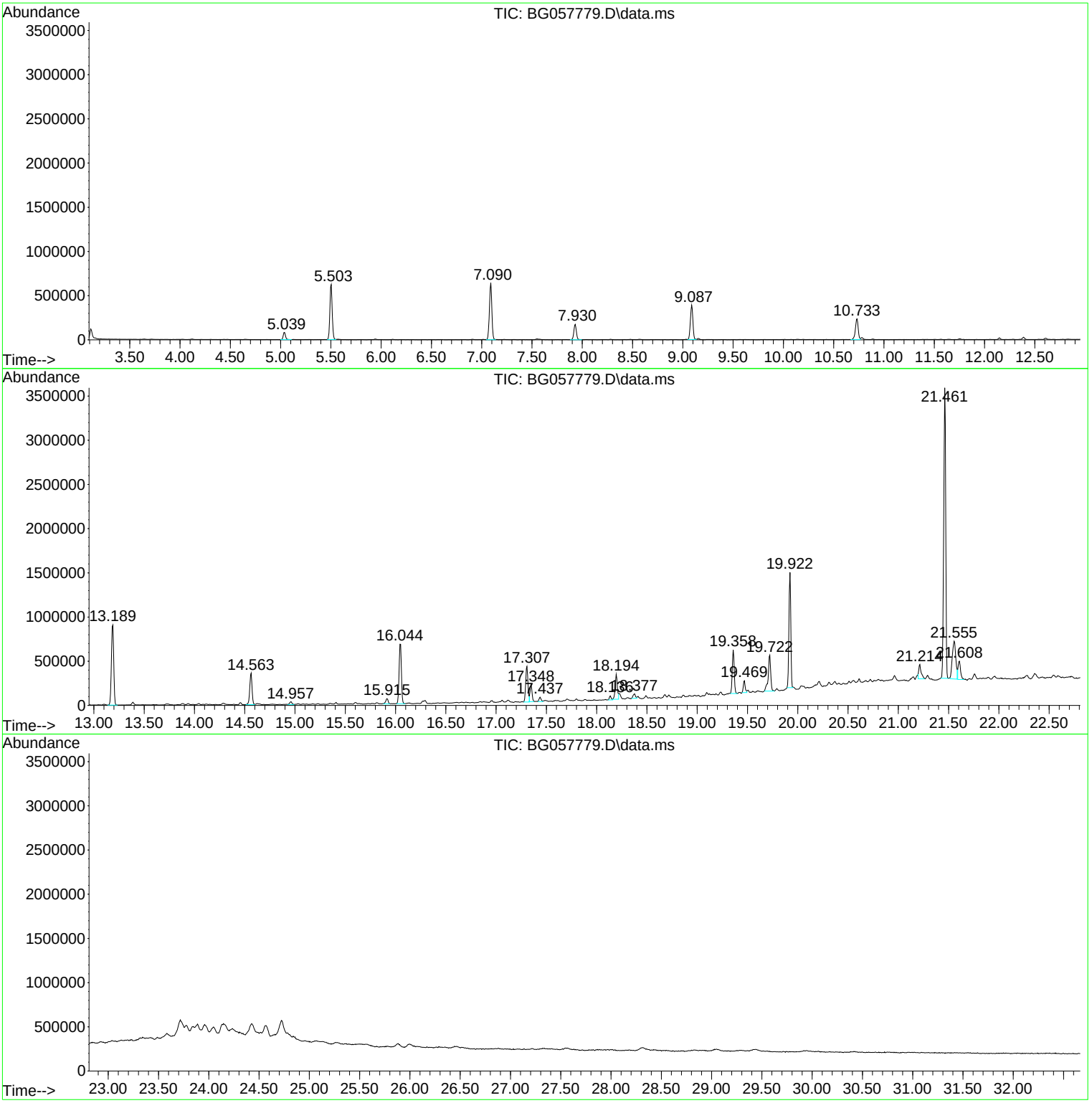
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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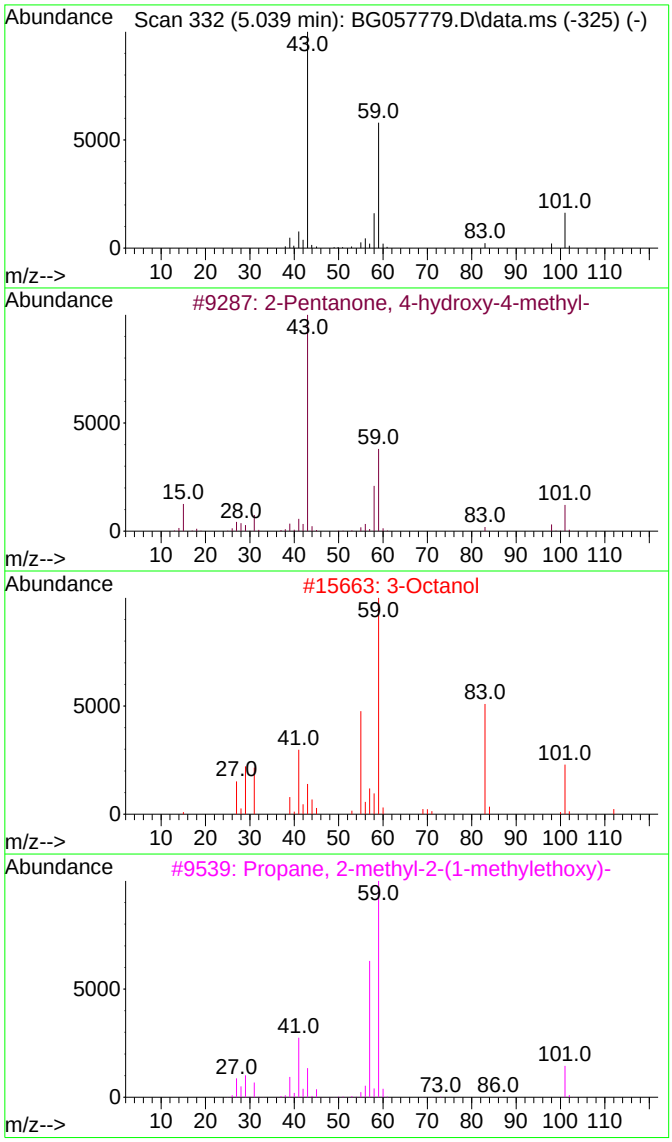
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

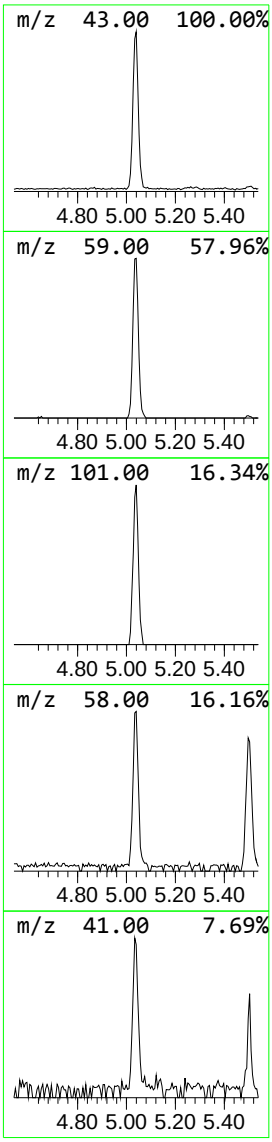
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.039	8.64 ng	131312	1,4-Dichlorobenzene-d4	7.930

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Octanol	130	C8H18O	000589-98-0	36
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





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Instrument :
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COMPOSIT-SB-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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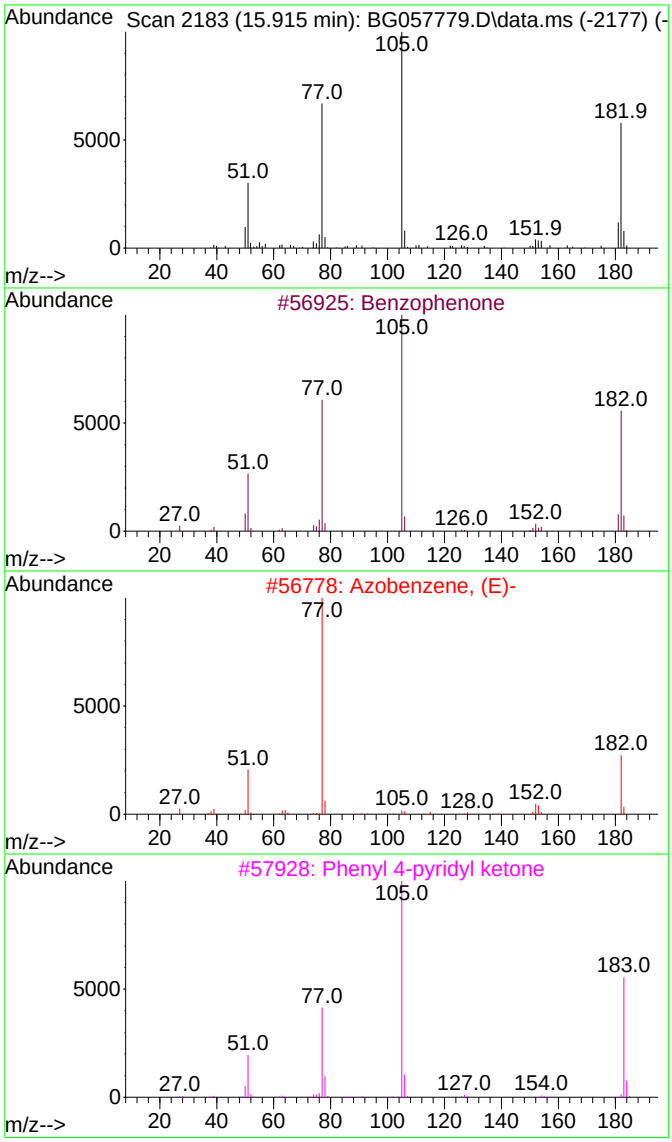
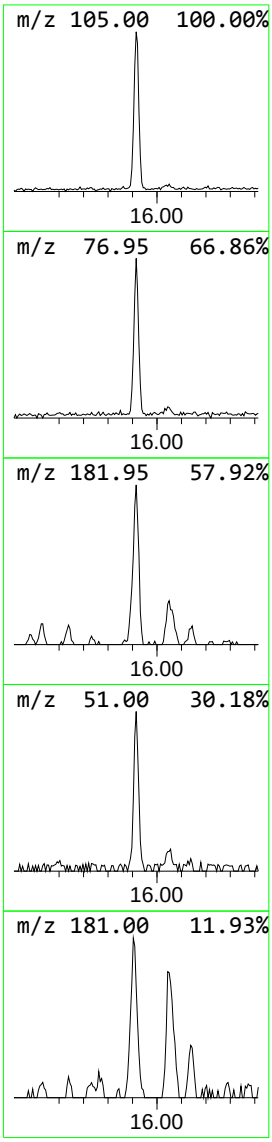
****

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.915	3.39 ng	94826	Acenaphthene-d10	14.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	95
2	Azobenzene, (E)-	182	C12H10N2	017082-12-1	59
3	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	49
4	Benzoylformic acid	150	C8H6O3	000611-73-4	49
5	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46





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ClientSampleId :
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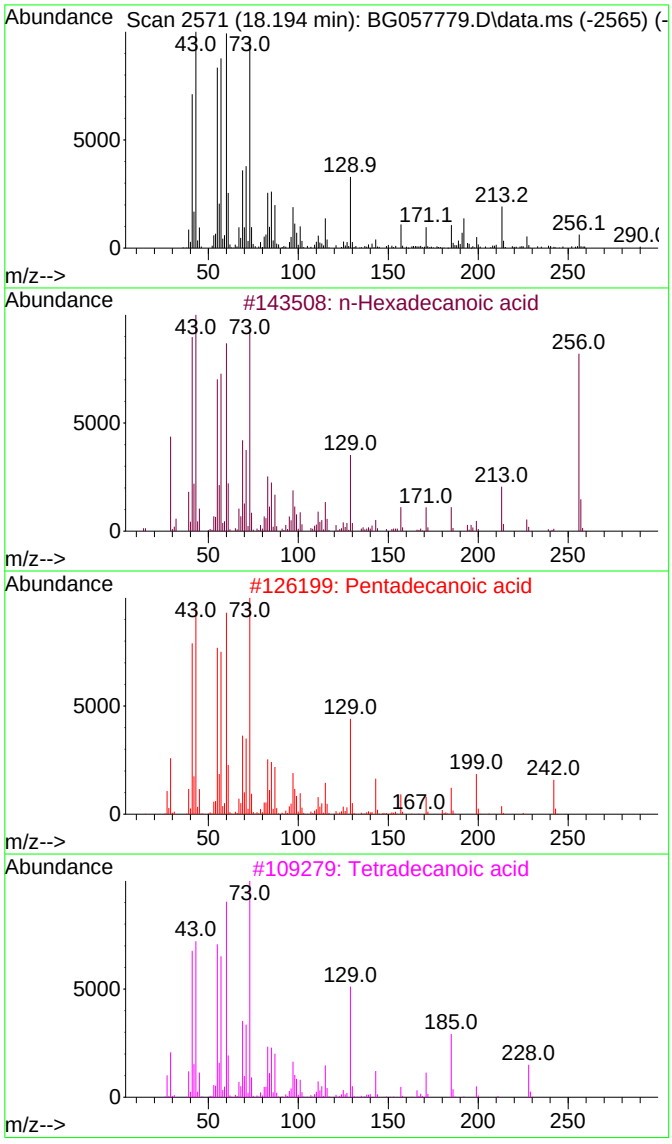
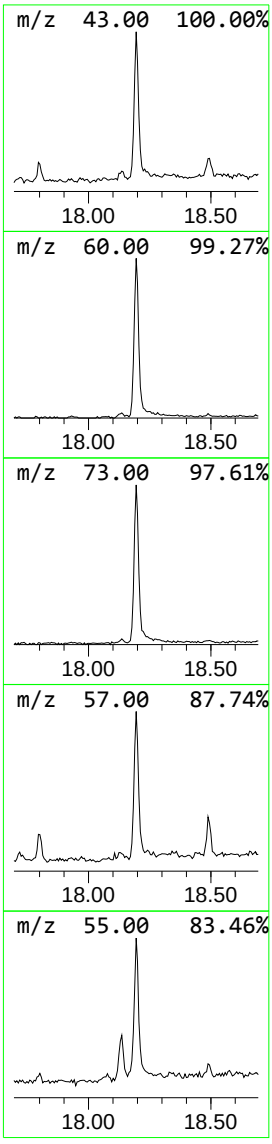
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.195	13.24 ng	413753	Phenanthrene-d10	17.307

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	68





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Misc :
ALS Vial : 14 Sample Multiplier: 1

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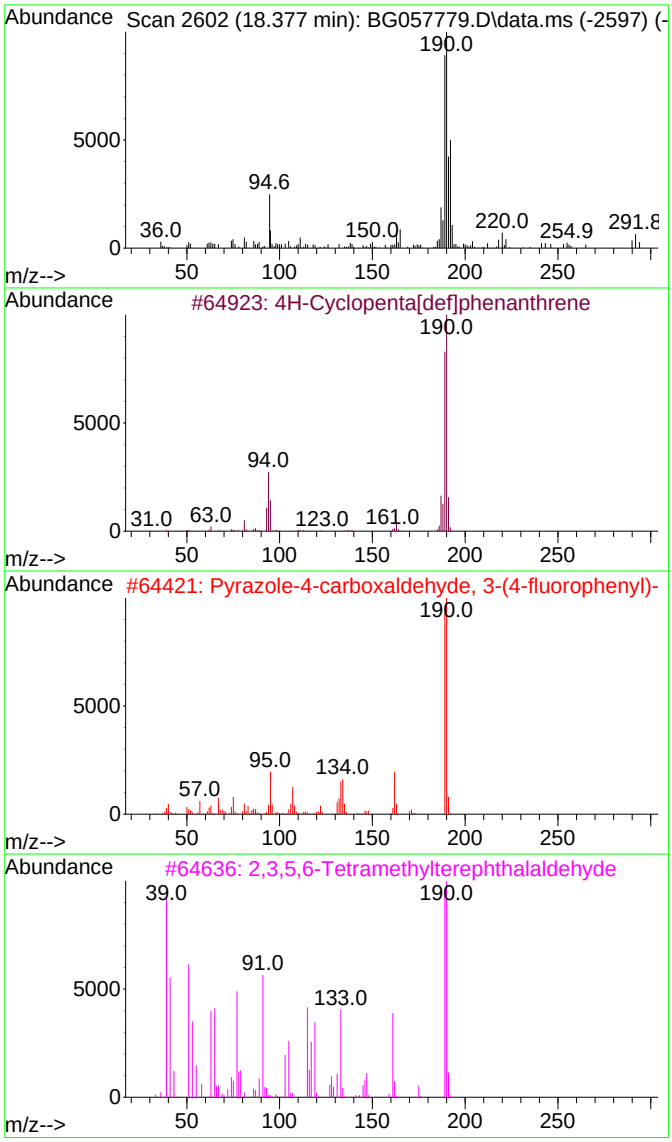
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

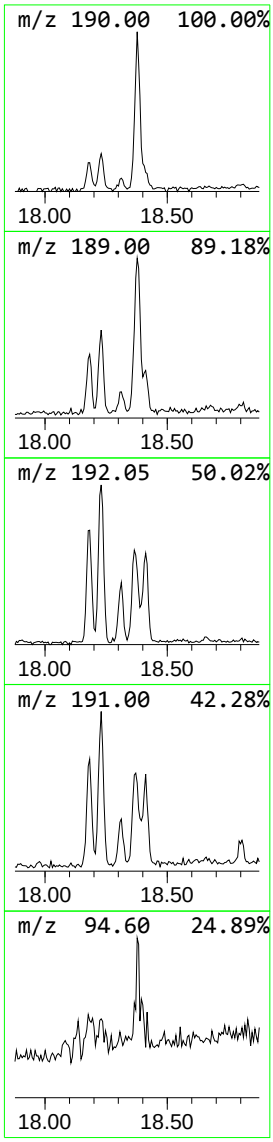
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.377	2.72 ng	85139	Phenanthrene-d10	17.307

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	86
2	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	43
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	43
4	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	40
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40





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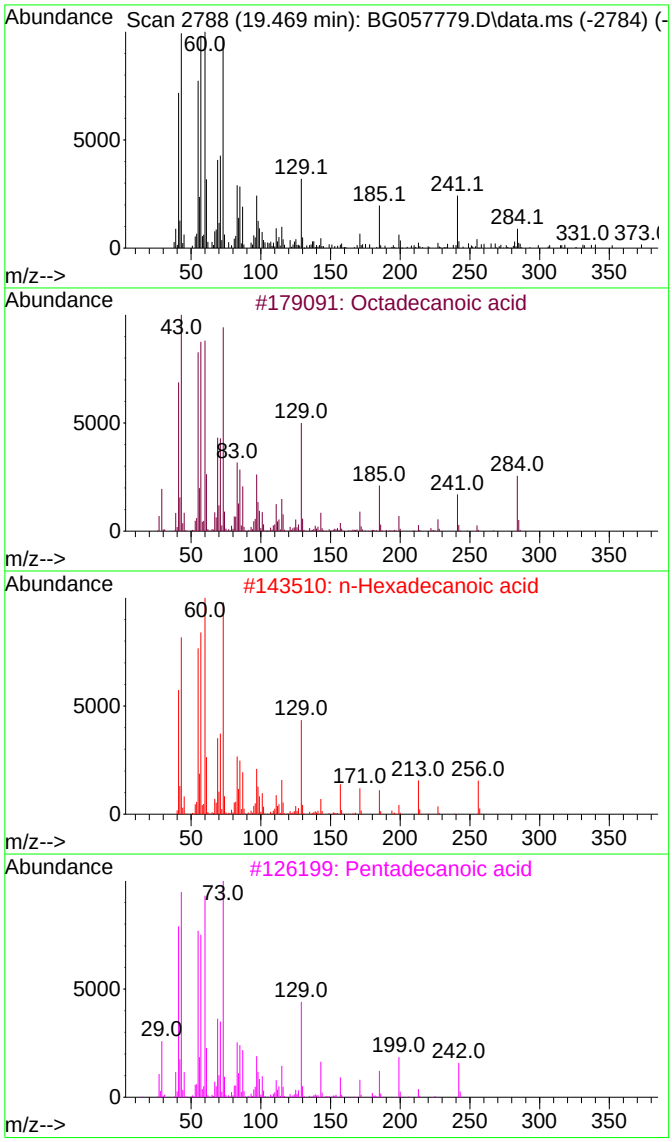
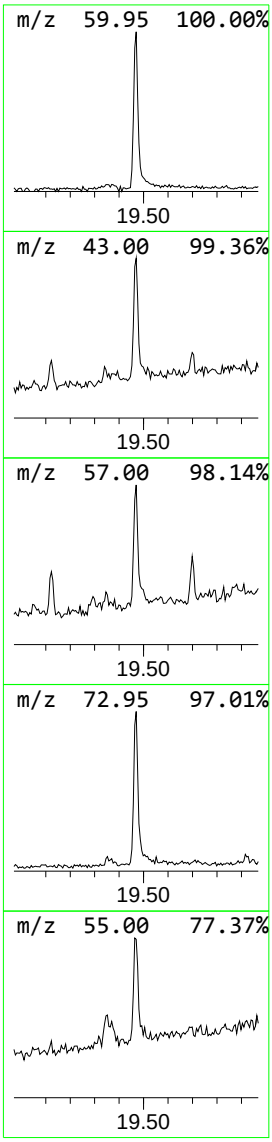
****

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.469	3.37 ng	174521	Chrysene-d12	21.561

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	80





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TIC Library : C:\Database\NIST20.L
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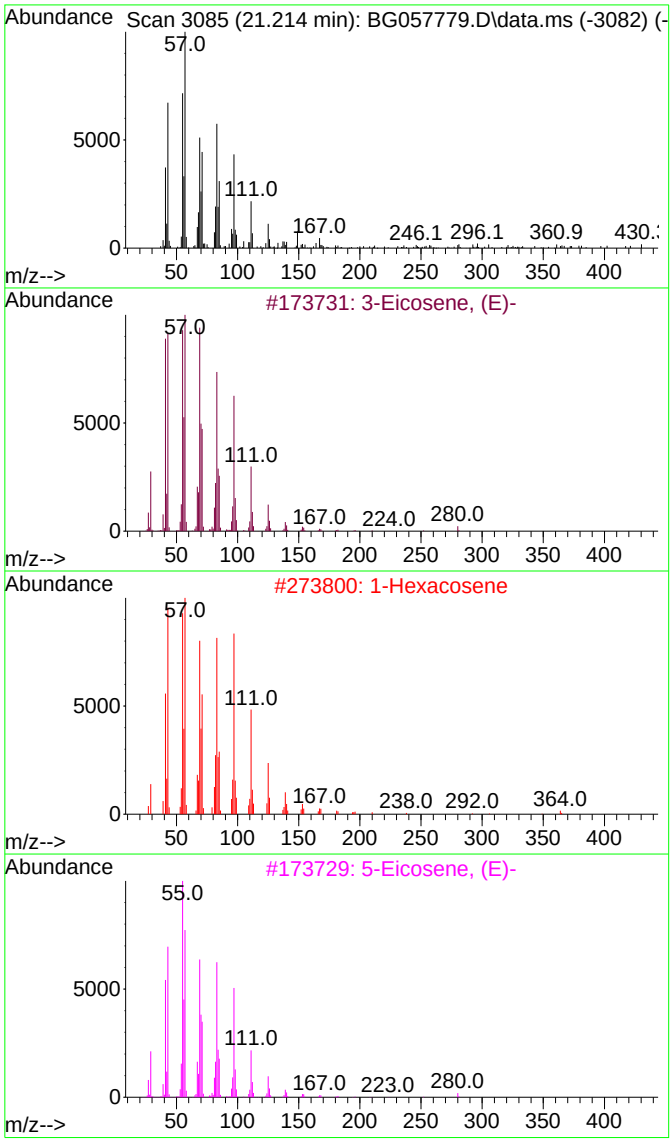
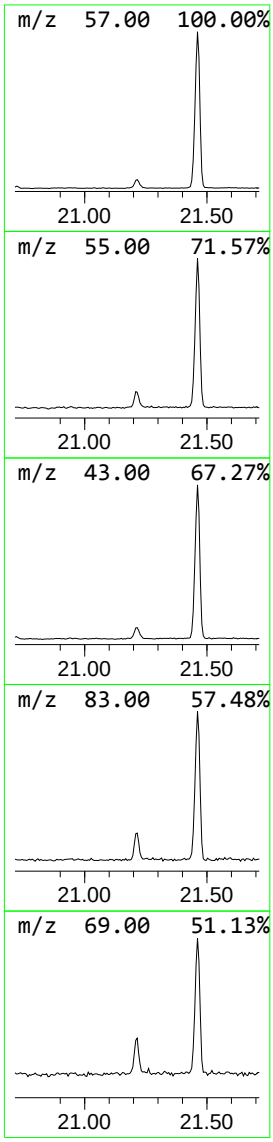
****

Peak Number 6 3-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.214	5.12 ng	265478	Chrysene-d12	21.561

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	94
2	1-Hexacosene	364	C26H52	018835-33-1	93
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	92
4	17-Pentatriacontene	491	C35H70	006971-40-0	91
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91





Tentatively Identified Compound (LSC) summary

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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-...	5.039	8.6	ng	131312	1	7.930	304098	20.0
Benzophenone	15.915	3.4	ng	94826	3	14.563	559956	20.0
n-Hexadecanoic ...	18.195	13.2	ng	413753	4	17.307	625200	20.0
4H-Cyclopenta[d...	18.377	2.7	ng	85139	4	17.307	625200	20.0
Octadecanoic acid	19.469	3.4	ng	174521	5	21.561	1036380	20.0
3-Eicosene, (E)-	21.214	5.1	ng	265478	5	21.561	1036380	20.0