LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122223\
Data File : BG060136.D
Acq On : 22 Dec 2023 13:29
Operator : MA/JU
Sample : 05898-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SD-73

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-BG122123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060136.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.118	3	5	20	rVB	383782	611257	5.16%	1.001%
2	5.045	325	333	341	rBV2	117498	207720	1.75%	0.340%
3	5.515	406	413	426	rBV	2223581	3809552	32.15%	6.241%
4	7.101	675	683	702	rBV	2643989	4616137	38.95%	7.562%
5	7.941	817	826	833	rBV	634364	1101908	9.30%	1.805%
6	9.099	1015	1023	1039	rBV	1484000	2686812	22.67%	4.401%
7	10.744	1295	1303	1316	rBV	960649	1767236	14.91%	2.895%
8	13.200	1713	1721	1733	rBV	4686517	7354401	62.06%	12.047%
9	14.575	1949	1955	1964	rBV	1989529	3112022	26.26%	5.098%
10	16.067	2201	2209	2224	rBV	3978131	6269617	52.91%	10.270%
11	17.325	2416	2423	2434	rBV	2950030	4368591	36.86%	7.156%
12	18.218	2570	2575	2585	rBV	439709	697631	5.89%	1.143%
13	19.945	2863	2869	2882	rBV	8860385	11850292	100.00%	19.412%
14	20.973	3040	3044	3049	rBV2	152937	170569	1.44%	0.279%
15	21.243	3084	3090	3102	rVB	1811950	2437244	20.57%	3.993%
16	21.590	3142	3149	3157	rBV	2298444	3671535	30.98%	6.014%
17	21.784	3178	3182	3187	rVB3	109302	163239	1.38%	0.267%
18	22.148	3238	3244	3252	rVB2	524500	881929	7.44%	1.445%
19	22.383	3279	3284	3297	rVB	753703	1339392	11.30%	2.194%
20	23.864	3531	3536	3541	rBV2	130143	214096	1.81%	0.351%
21	23.917	3542	3545	3556	rVB5	112079	249083	2.10%	0.408%
22	24.763	3679	3689	3702	rVB2	1224324	3464875	29.24%	5.676%

Sum of corrected areas: 61045138

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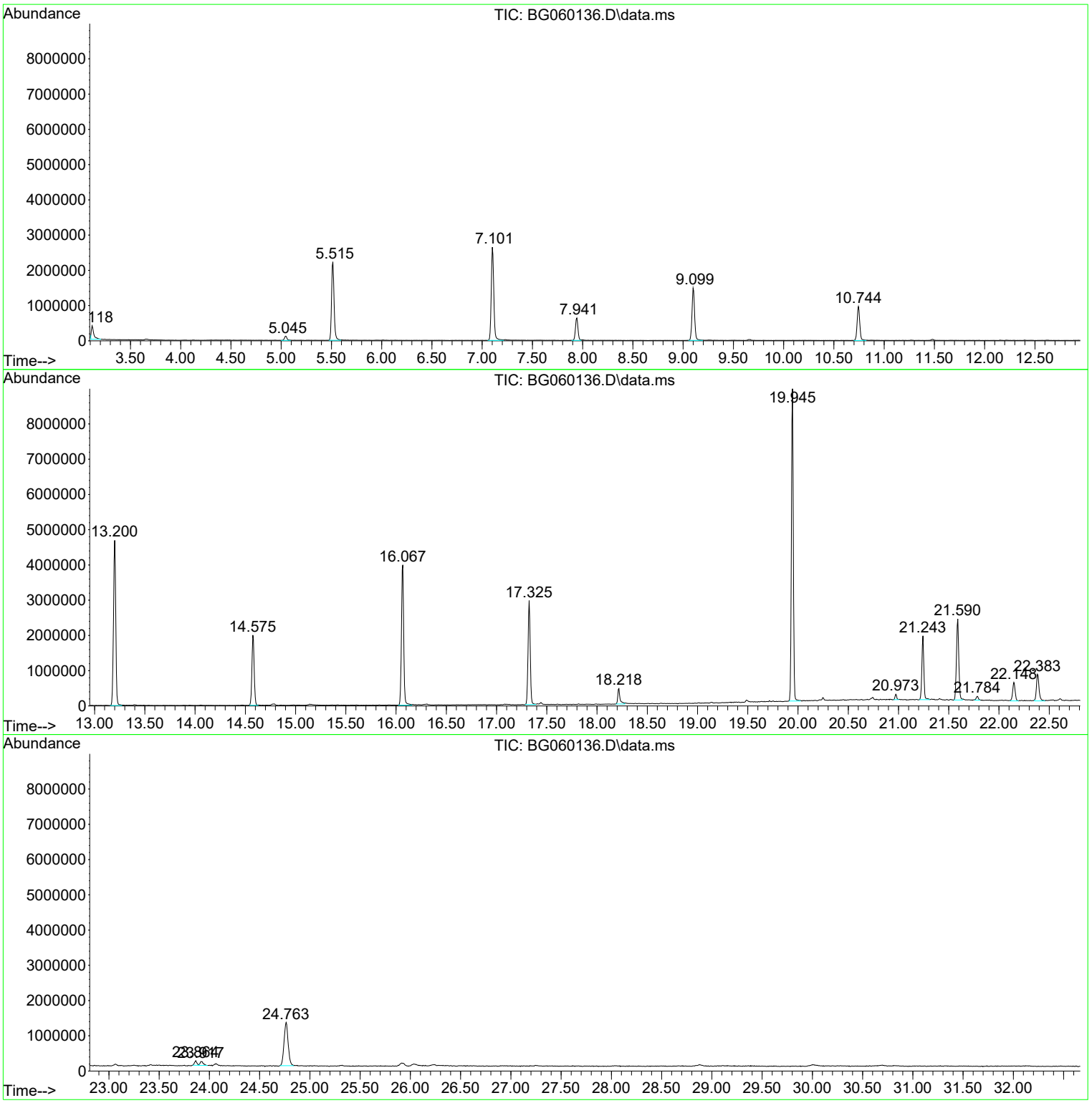
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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
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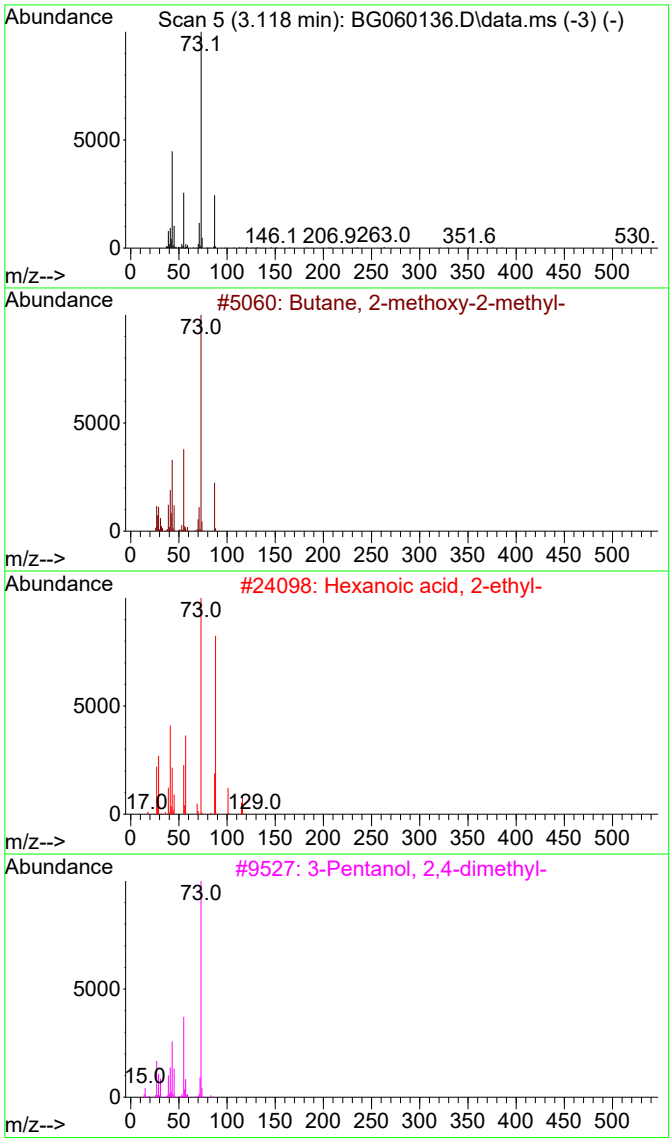
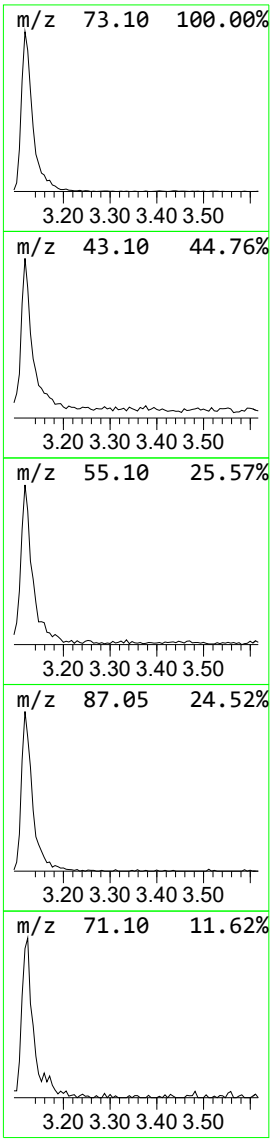
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.118	11.09 ng	611257	1,4-Dichlorobenzene-d4	7.941

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	50
2	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	33
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	1-Propene-1-thiol	74	C3H6S	000925-89-3	22





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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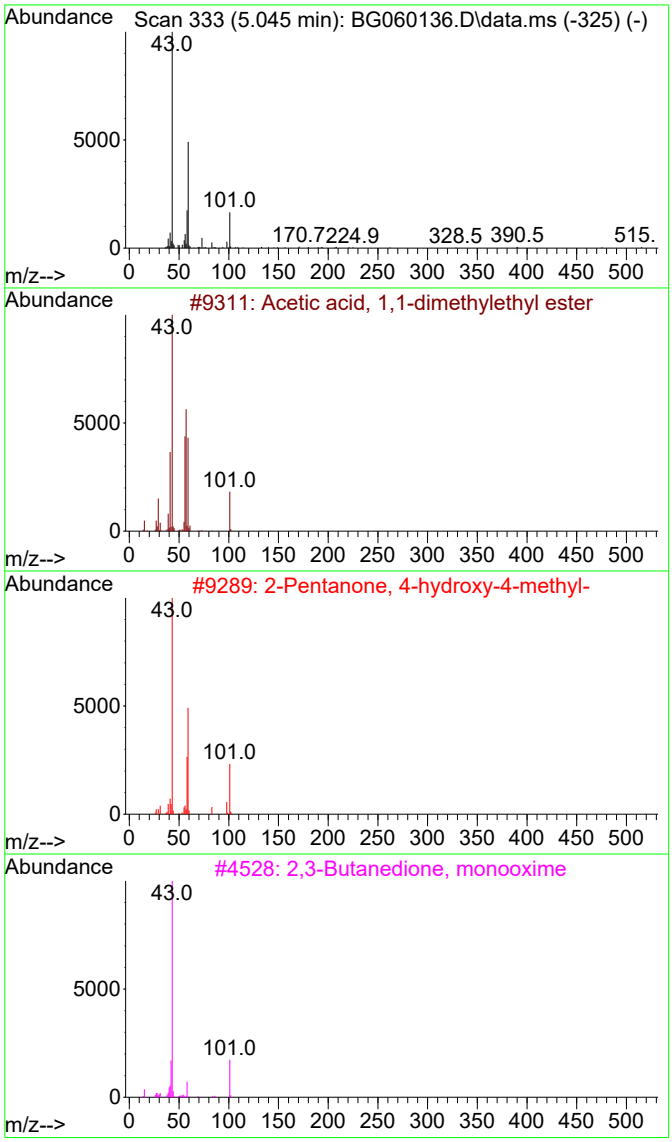
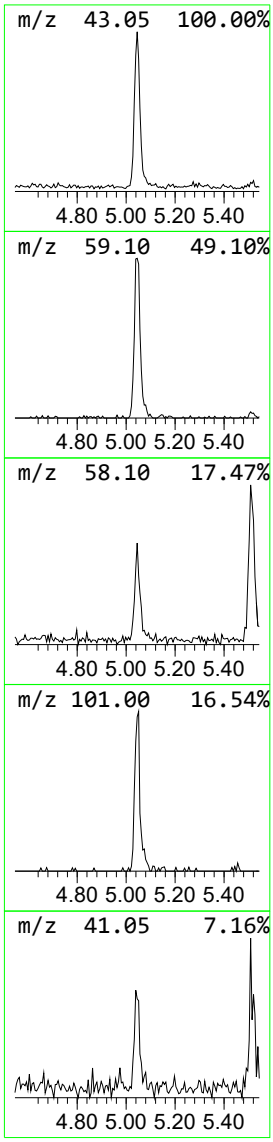
****
Peak Number 2 Acetic acid, 1,1-dimethylet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.045	3.77 ng	207720	1,4-Dichlorobenzene-d4	7.941

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	59
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Acetone	58	C3H6O	000067-64-1	9





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
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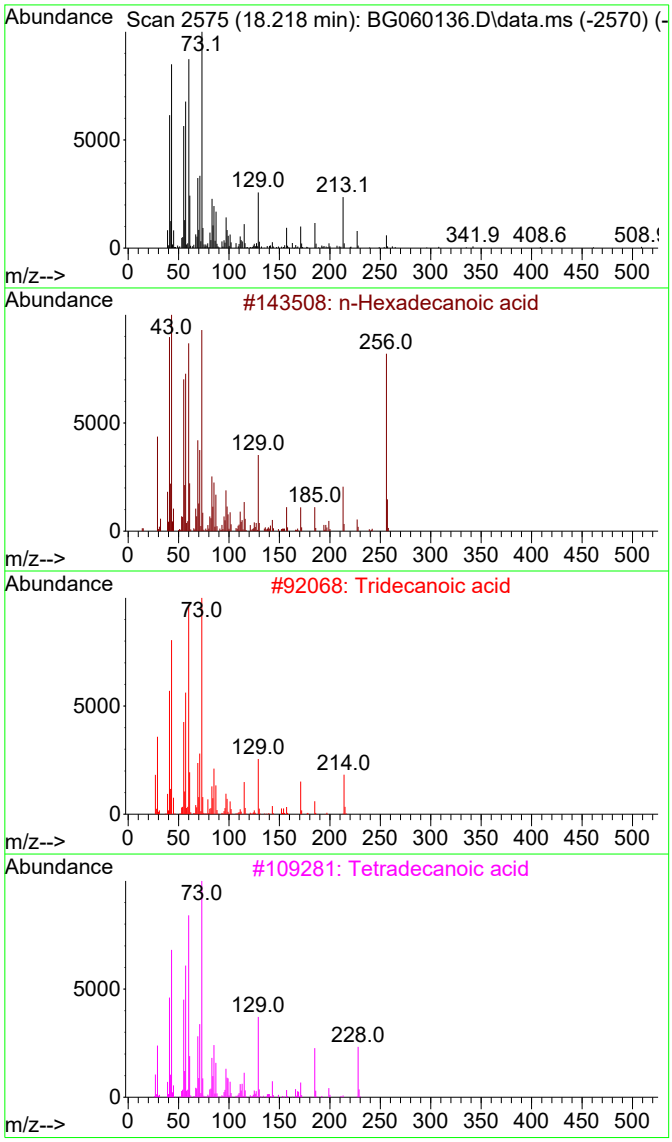
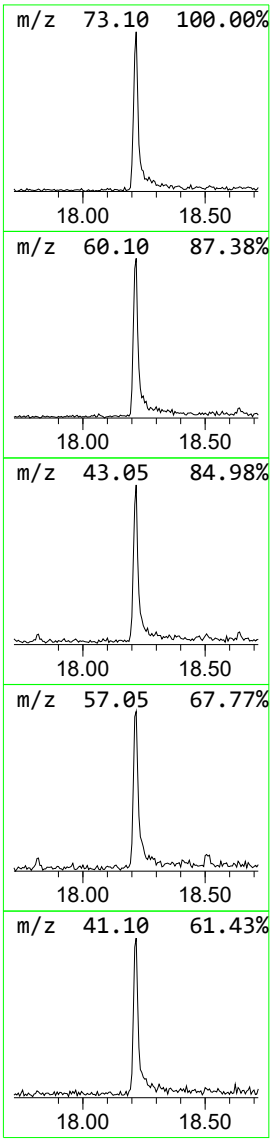
Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.218	3.19 ng	697631	Phenanthrene-d10	17.325

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





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TIC Library : C:\Database\NIST20.L
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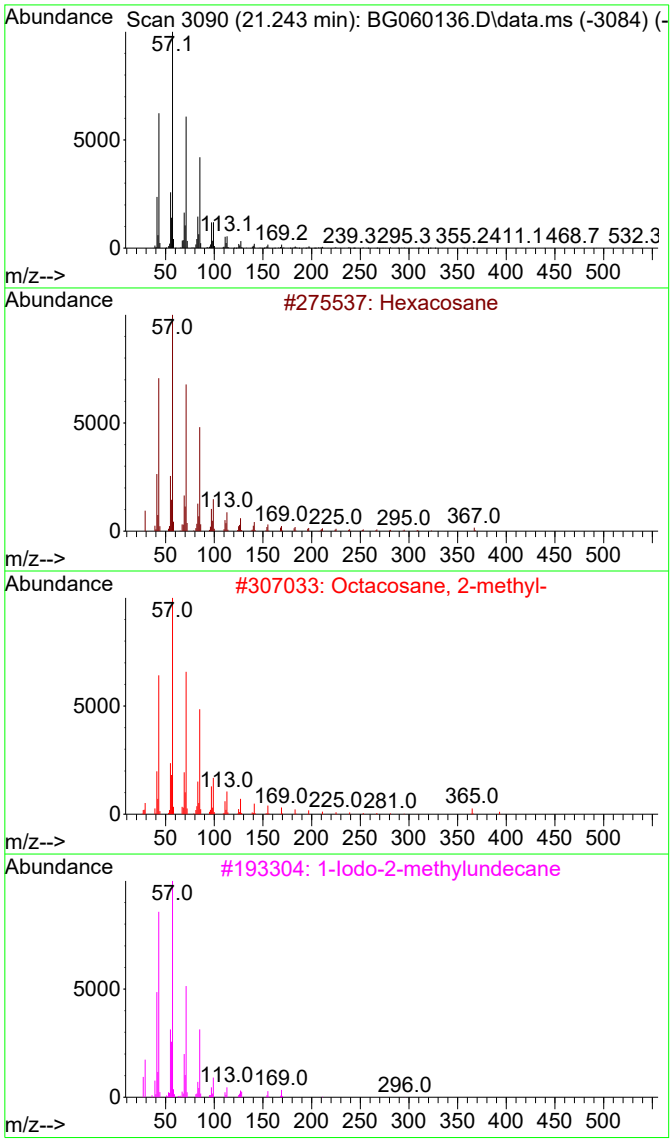
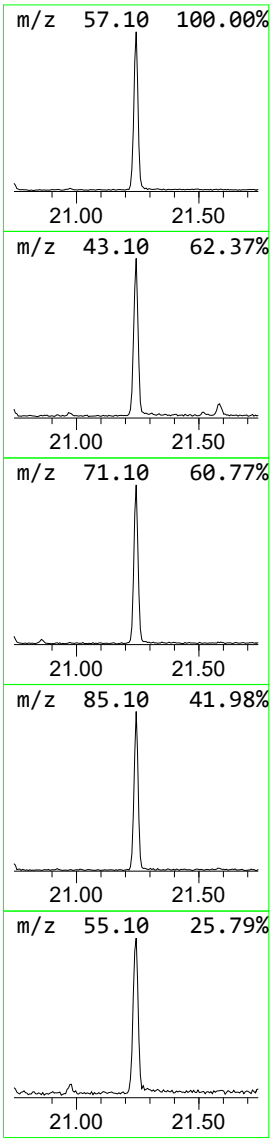
Peak Number 4 Hexacosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.243	13.28 ng	2437240	Chrysene-d12	21.590

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
3	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	87
4	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	81
5	Hentriacontane	437	C31H64	000630-04-6	80





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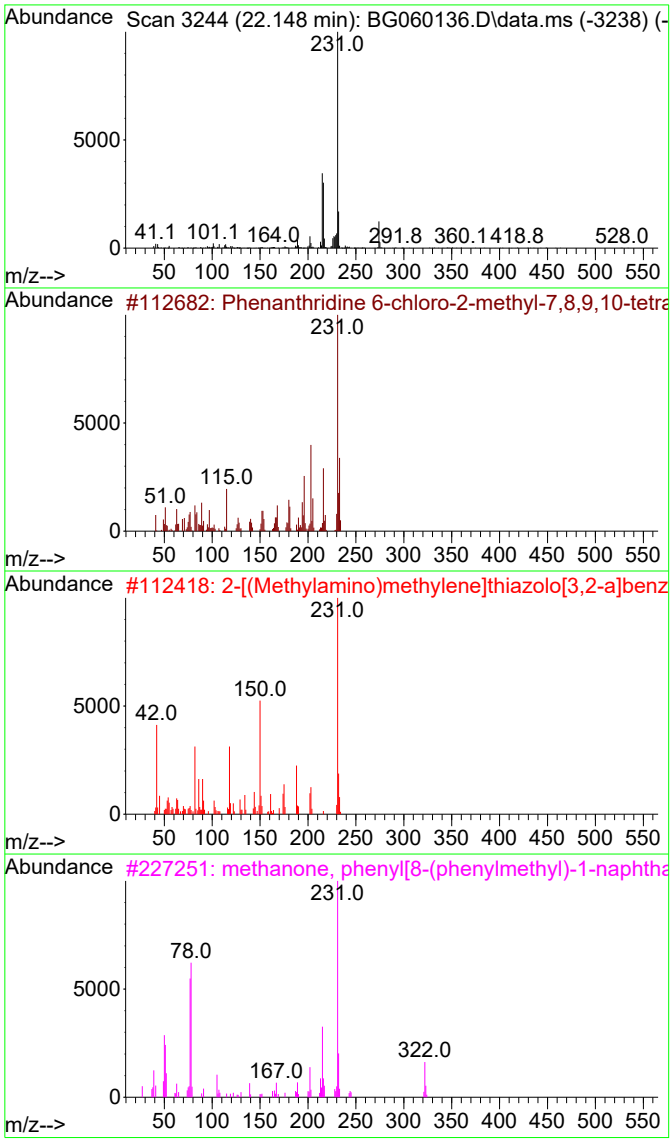
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

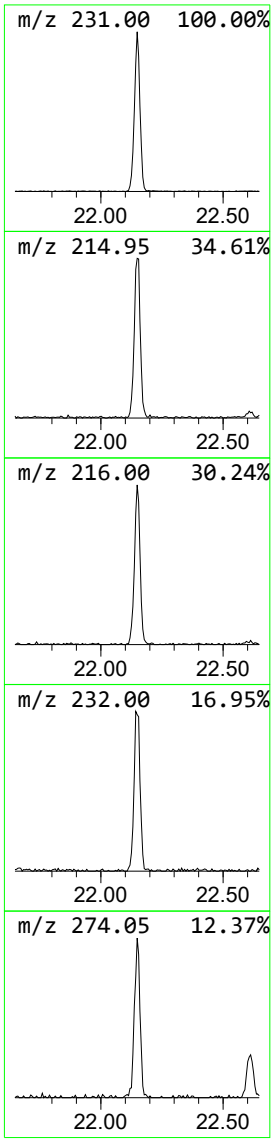
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Phenanthridine 6-chloro-2-m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.148	4.80 ng	881929	Chrysene-d12	21.590

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthridine 6-chloro-2-methyl...	231	C14H14ClN	035417-77-7	53
2	2-[(Methylamino)methylene]thiazo...	231	C11H9N3OS	072740-41-1	49
3	methanone, phenyl[8-(phenylmethy...	322	C24H18O	1000402-34-2	45
4	(1Alpha,7beta,9aalpha)-4-(3-fury...	231	C15H21NO	003606-26-6	40
5	Phthalic acid, 2,2,2-trifluoroet...	346	C17H21F3O4	1000370-99-7	38





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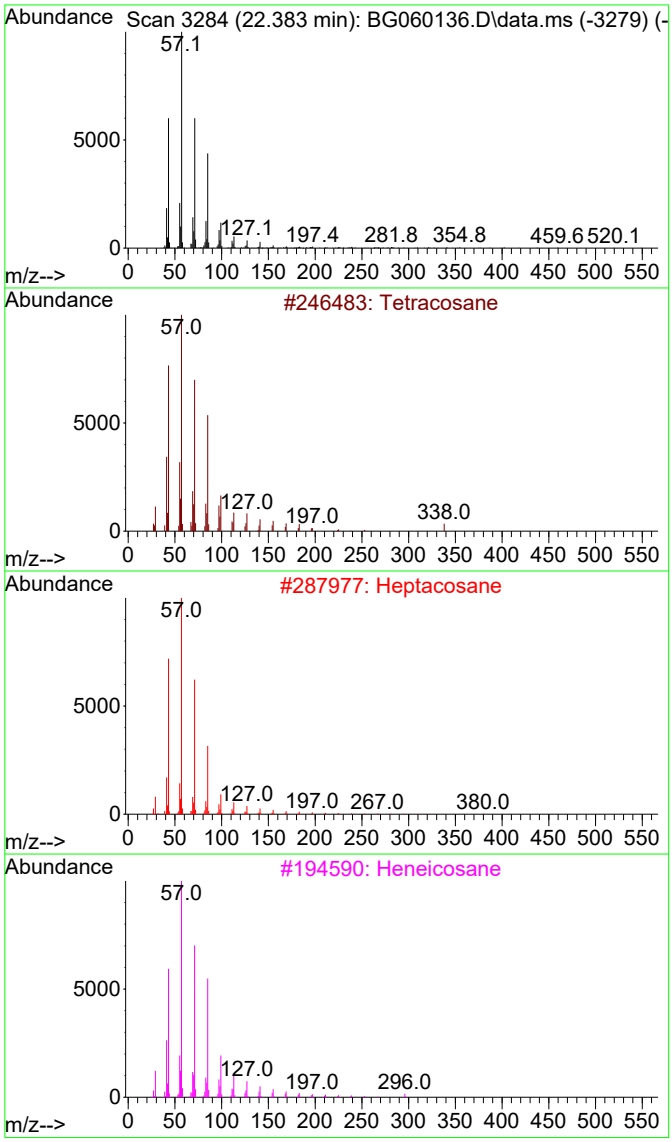
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

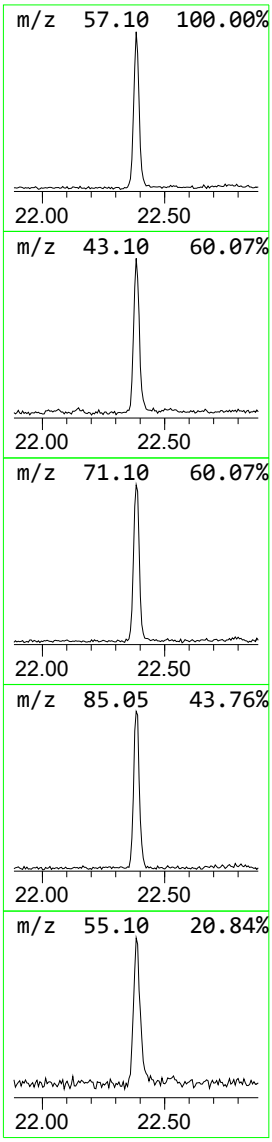
****

Peak Number 6 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.383	7.30 ng	1339390	Chrysene-d12	21.590

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	95
2	Heptacosane	380	C27H56	000593-49-7	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	90
5	Nonadecane	268	C19H40	000629-92-5	90





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
Butane, 2-metho...	3.118	11.1	ng	611257	1	7.941	1101910	20.0
Acetic acid, 1,...	5.045	3.8	ng	207720	1	7.941	1101910	20.0
n-Hexadecanoic ...	18.218	3.2	ng	697631	4	17.325	4368590	20.0
Hexacosane	21.243	13.3	ng	2437240	5	21.590	3671540	20.0
Phenanthridine ...	22.148	4.8	ng	881929	5	21.590	3671540	20.0
Tetracosane	22.383	7.3	ng	1339390	5	21.590	3671540	20.0