LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG013024\
Data File : BG060479.D
Acq On : 30 Jan 2024 11:48
Operator : MA/JU
Sample : PB158676BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB158676BL

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-BG010824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060479.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.499	401	410	424	rBV	3664786	5862245	28.76%	6.445%
2	7.092	674	681	699	rBV	3704337	6442021	31.60%	7.082%
3	7.920	815	822	833	rBV	633296	1110090	5.45%	1.220%
4	9.083	1012	1020	1041	rBV	2342114	4337754	21.28%	4.769%
5	10.723	1292	1299	1312	rBV	933031	1694841	8.31%	1.863%
6	13.184	1707	1718	1733	rBV	7200088	11808259	57.93%	12.981%
7	14.559	1945	1952	1964	rBV	1944972	2893568	14.20%	3.181%
8	16.052	2198	2206	2234	rBV	6024508	9487117	46.54%	10.429%
9	17.309	2412	2420	2431	rBV	2762720	4172696	20.47%	4.587%
10	19.618	2806	2813	2823	rVB2	215554	322567	1.58%	0.355%
11	19.930	2859	2866	2877	rBV	13893080	20383074	100.00%	22.408%
12	20.658	2986	2990	2994	rBV2	204389	222481	1.09%	0.245%
13	21.569	3138	3145	3157	rBV2	3046038	5089132	24.97%	5.595%
14	22.344	3272	3277	3284	rVB2	203871	326642	1.60%	0.359%
15	22.532	3299	3309	3320	rVB5	83695	338830	1.66%	0.372%
16	23.026	3385	3393	3402	rVB	469607	913952	4.48%	1.005%
17	23.813	3519	3527	3539	rVB	592572	1267873	6.22%	1.394%
18	24.736	3672	3684	3697	rBV2	2495380	6974748	34.22%	7.668%
19	25.840	3860	3872	3886	rBV2	664331	1963072	9.63%	2.158%
20	27.162	4084	4097	4112	rBV2	578559	2067997	10.15%	2.273%
21	28.760	4356	4369	4387	rVB3	372729	1601283	7.86%	1.760%
22	30.687	4682	4697	4710	rBV5	309278	1684398	8.26%	1.852%

Sum of corrected areas: 90964640

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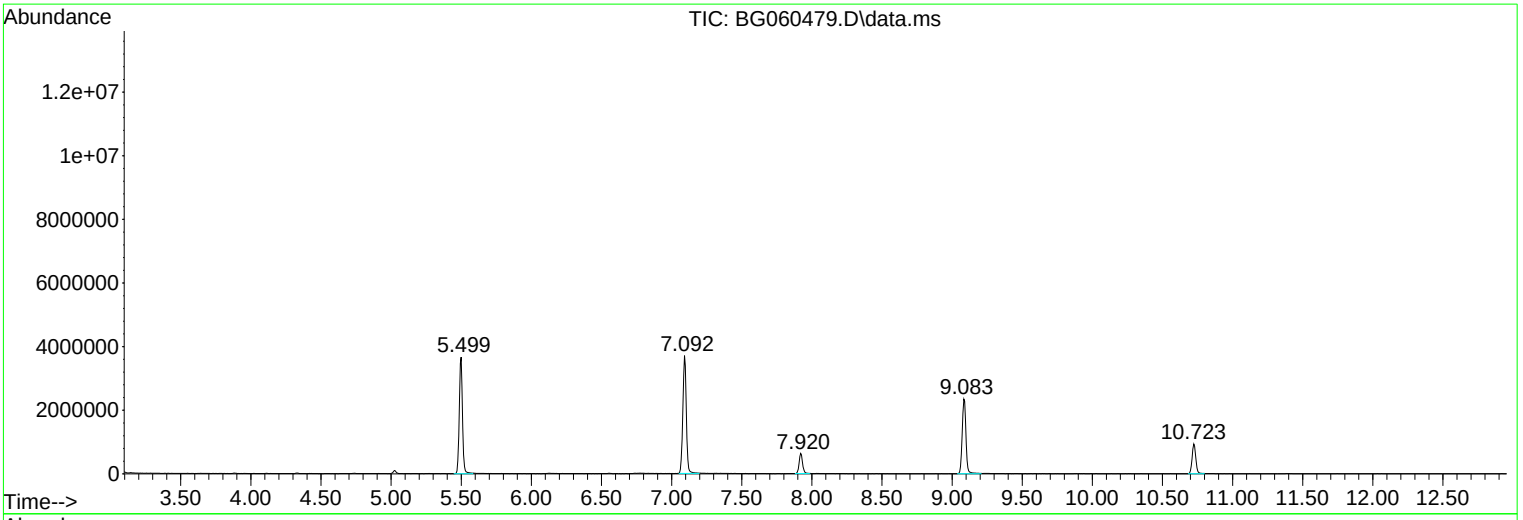
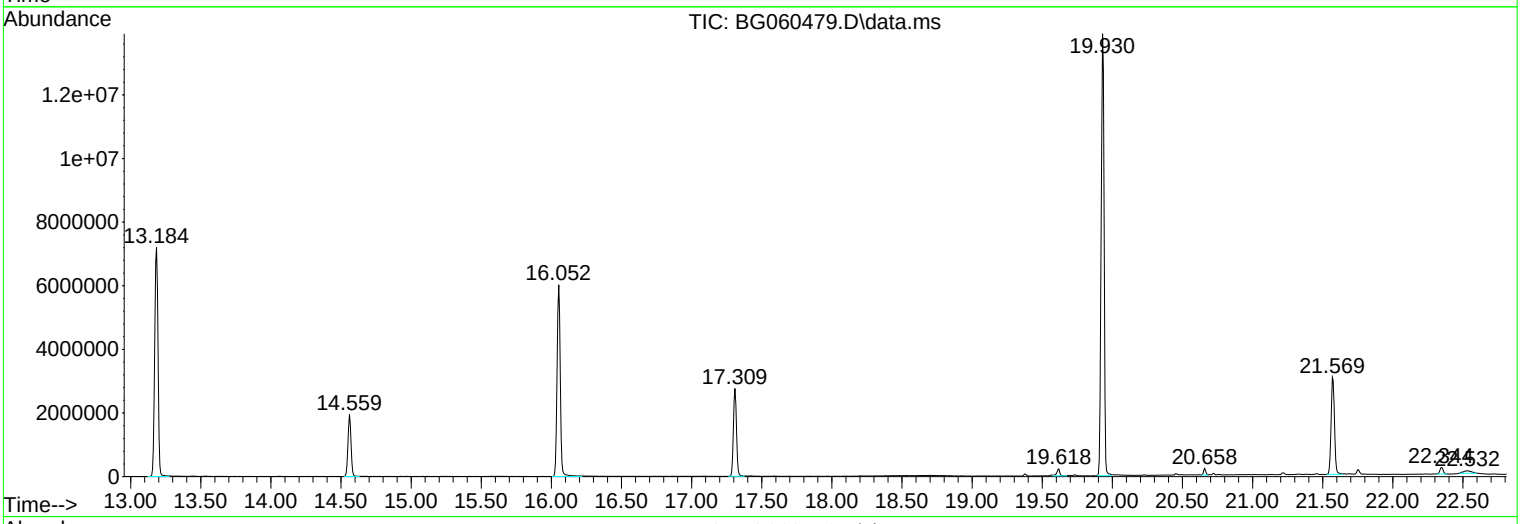
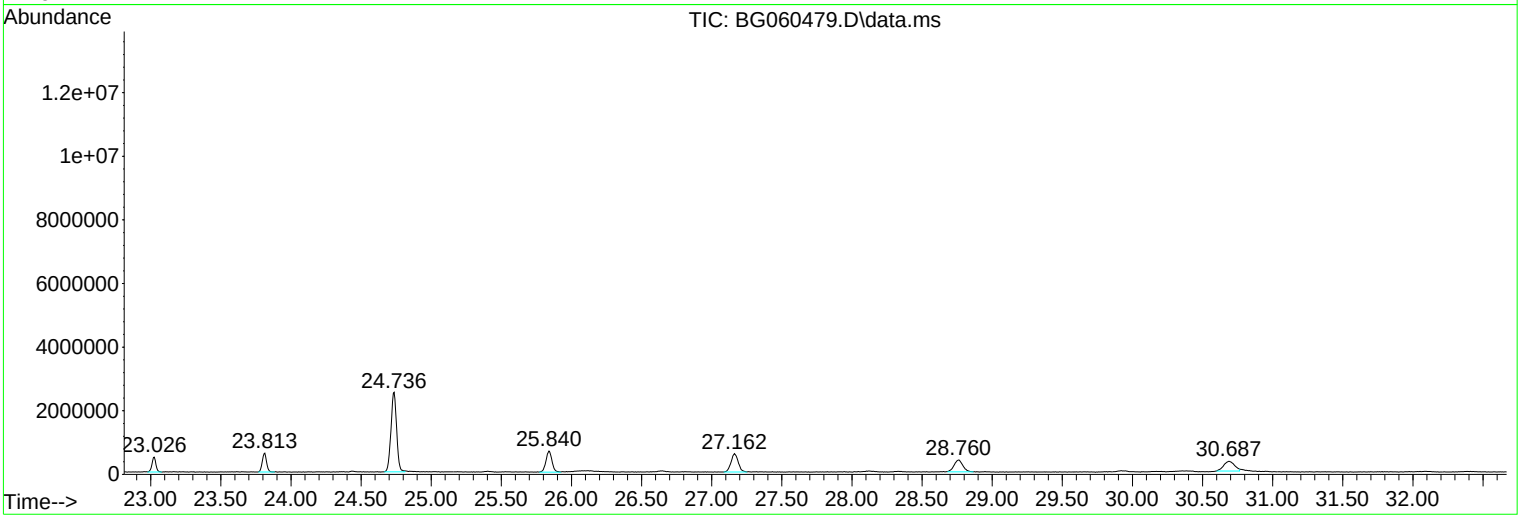
ClientSampleId :
PB158676BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.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

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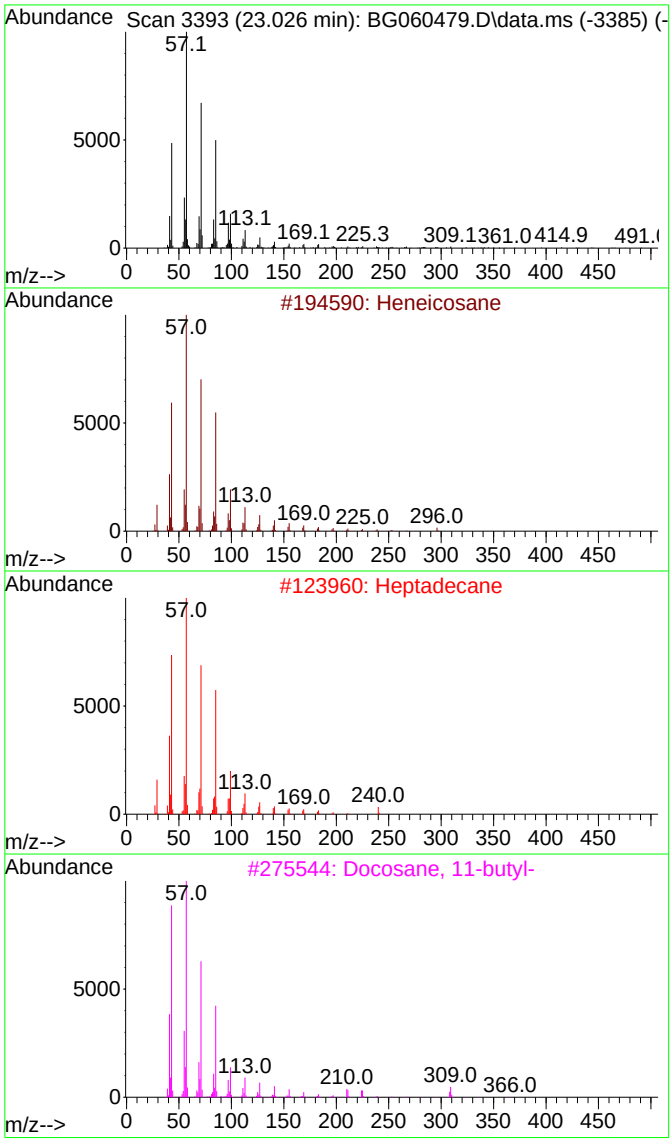
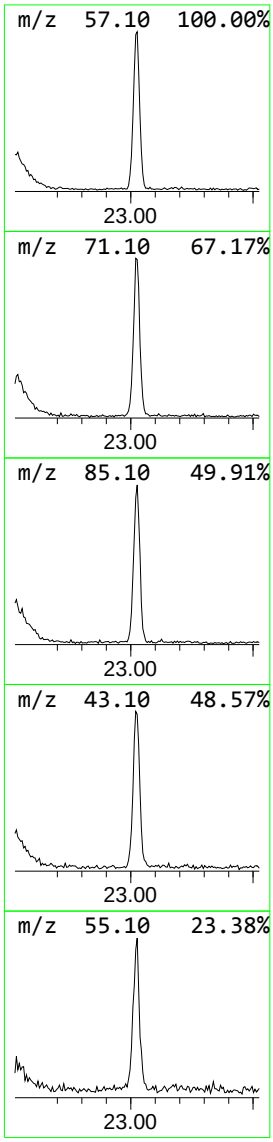
Peak Number 1 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.026	3.59 ng	913952	Chrysene-d12	21.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane	240	C17H36	000629-78-7	90
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	86
4	Hexadecane	226	C16H34	000544-76-3	80
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80





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ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
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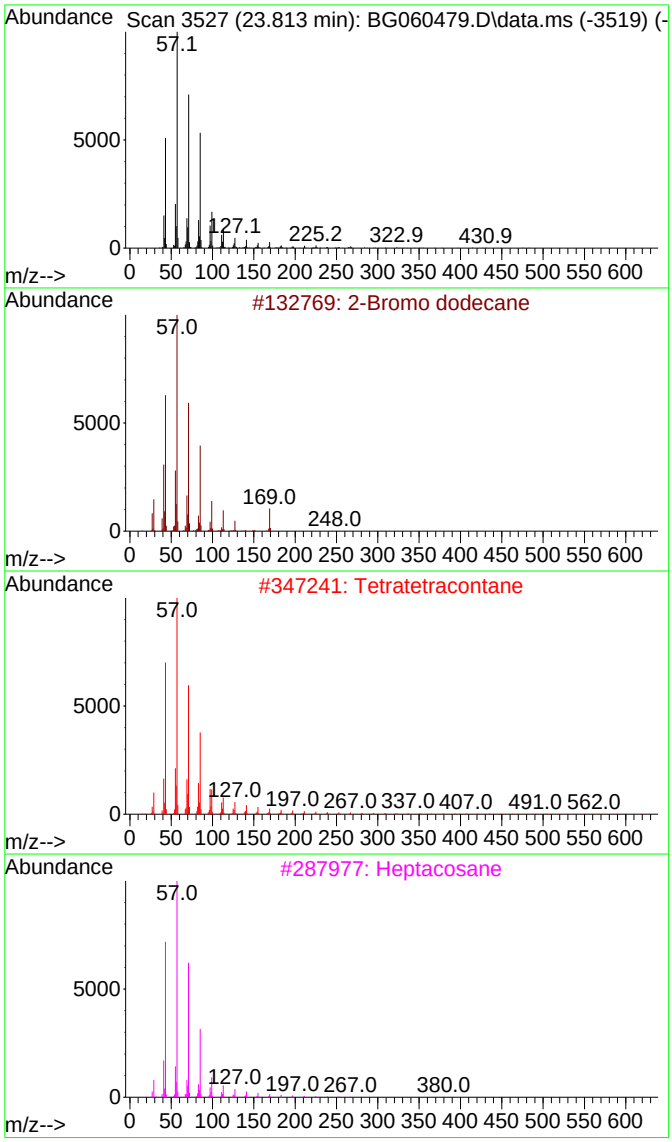
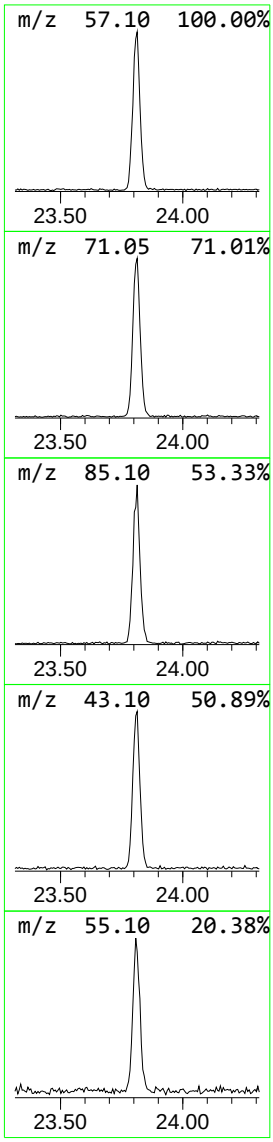
Peak Number 2 2-Bromo dodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.813	3.64 ng	1267870	Perylene-d12	24.730

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	76
2	Tetratetracontane	619	C44H90	007098-22-8	74
3	Heptacosane	380	C27H56	000593-49-7	72
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	68
5	Heneicosane	296	C21H44	000629-94-7	64





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Acq On : 30 Jan 2024 11:48
Operator : MA/JU
Sample : PB158676BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB158676BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
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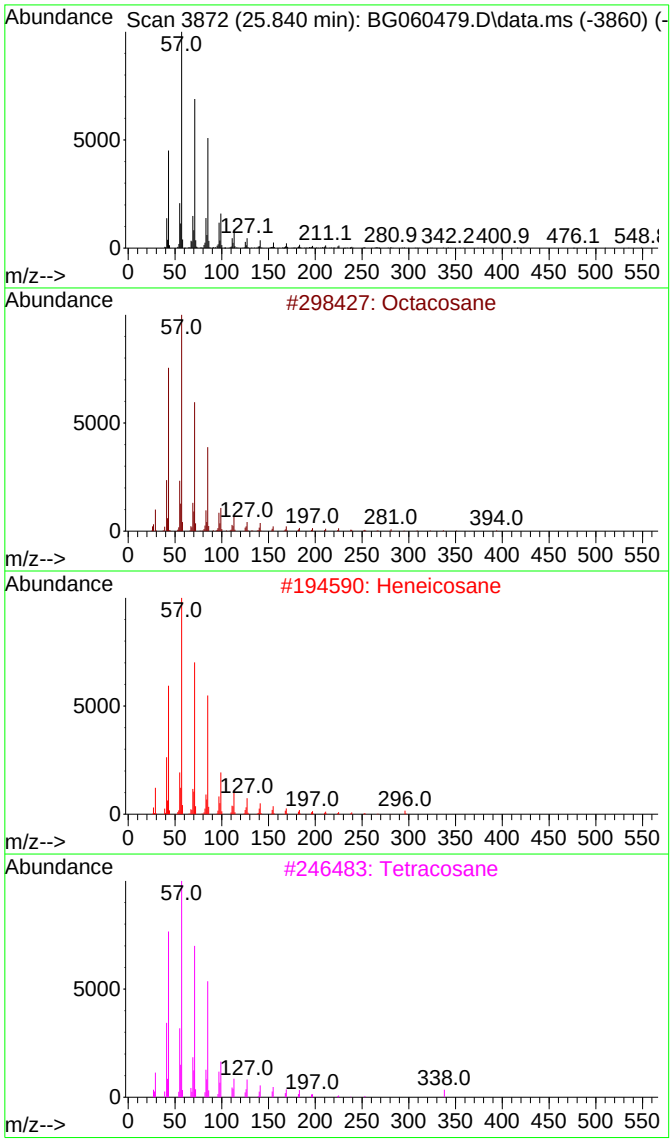
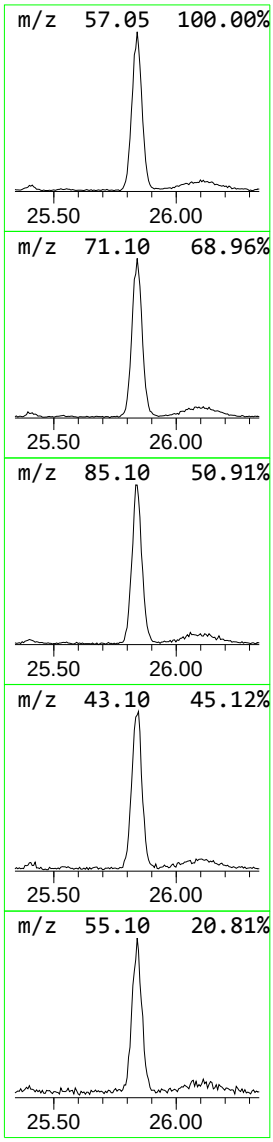
Peak Number 3 Octacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.840	5.63 ng	1963070	Perylene-d12	24.730

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	4-Methylheneicosane	310	C22H46	025117-29-7	90
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86





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Acq On : 30 Jan 2024 11:48
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Sample : PB158676BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB158676BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
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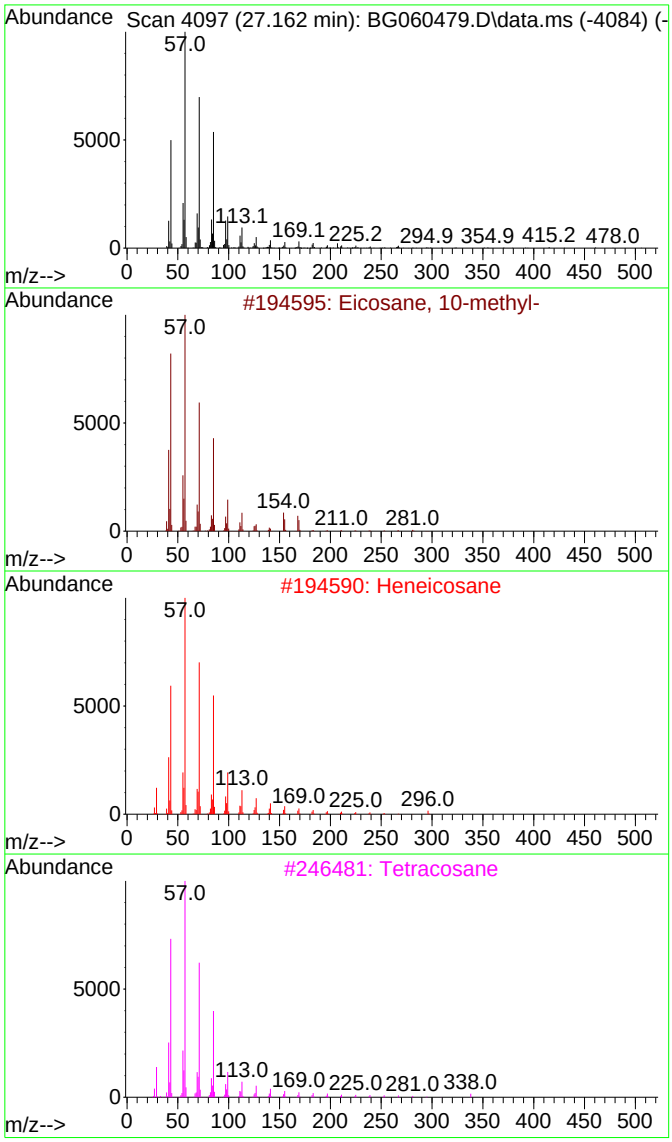
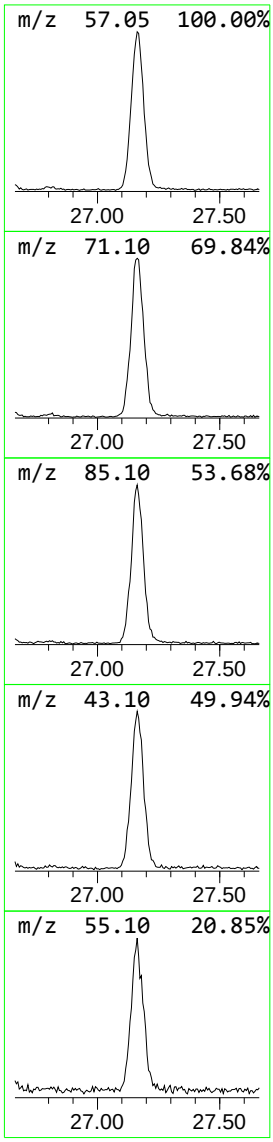
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Eicosane, 10-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.162	5.93 ng	2068000	Perylene-d12	24.730

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
2	Heneicosane	296	C21H44	000629-94-7	90
3	Tetracosane	338	C24H50	000646-31-1	87
4	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	86
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	86





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Operator : MA/JU
Sample : PB158676BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB158676BL

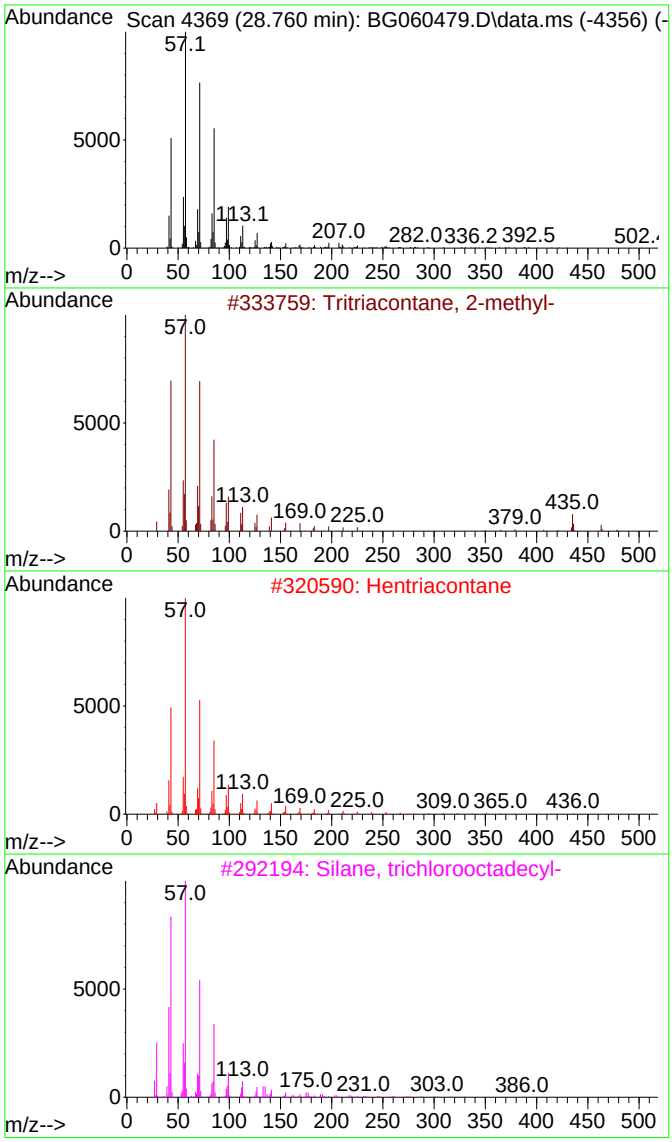
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

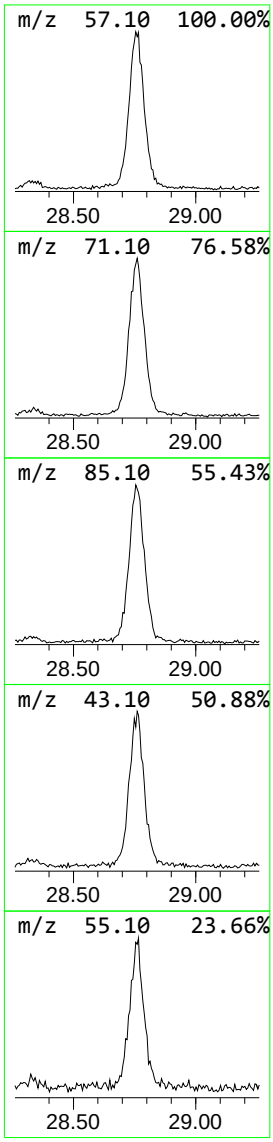
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Tritriacontane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.760	4.59 ng	1601280	Perylene-d12	24.730

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tritriacontane, 2-methyl-	479	C34H70	066214-27-5	90
2	Hentriacontane	437	C31H64	000630-04-6	80
3	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	72
4	Heptadecane, 3-methyl-	254	C18H38	006418-44-6	64
5	Heptacosane	380	C27H56	000593-49-7	64





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ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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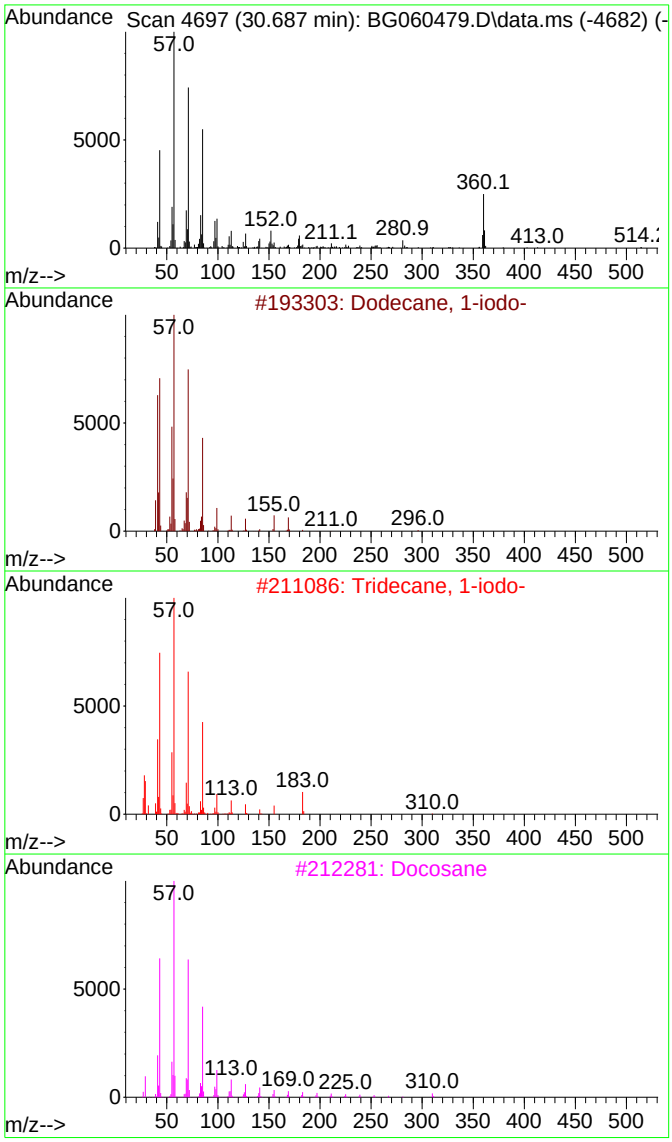
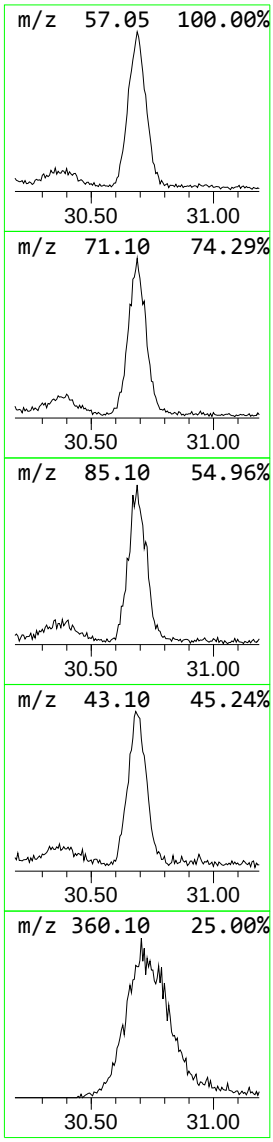
Peak Number 6 Dodecane, 1-iodo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.688	4.83 ng	1684400	Perylene-d12	24.730

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	68
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64
3	Docosane	310	C22H46	000629-97-0	64
4	Heptadecane	240	C17H36	000629-78-7	64
5	Nonadecane	268	C19H40	000629-92-5	64





Tentatively Identified Compound (LSC) summary

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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
Heneicosane	23.026	3.6	ng	913952	5	21.569	5089130	20.0
2-Bromo dodecane	23.813	3.6	ng	1267870	6	24.730	6974750	20.0
Octacosane	25.840	5.6	ng	1963070	6	24.730	6974750	20.0
Eicosane, 10-me...	27.162	5.9	ng	2068000	6	24.730	6974750	20.0
Tritriacontane,...	28.760	4.6	ng	1601280	6	24.730	6974750	20.0
Dodecane, 1-iodo-	30.688	4.8	ng	1684400	6	24.730	6974750	20.0