LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031424\
Data File : BF137590.D
Acq On : 14 Mar 2024 15:01
Operator : CG\JU
Sample : PB159568BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB159568BL

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_F\Methods\8270-BF022924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137590.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.945	482	486	497	rBV	174083	285898	4.39%	0.660%
2	5.345	549	554	574	rBV	5226366	6156207	94.57%	14.208%
3	6.369	722	728	748	rBV	4827855	6262412	96.21%	14.453%
4	6.722	785	788	808	rBV	1367184	1368377	21.02%	3.158%
5	7.292	880	885	888	rBV	3655751	3795717	58.31%	8.760%
6	8.004	1002	1006	1028	rBV	1832706	1818287	27.93%	4.196%
7	9.086	1184	1190	1193	rBV	6200704	6509350	100.00%	15.023%
8	9.757	1299	1304	1318	rBV	2299137	1991301	30.59%	4.596%
9	10.545	1434	1438	1465	rBV	3601123	3578381	54.97%	8.259%
10	11.239	1552	1556	1567	rBV	2116129	1850321	28.43%	4.270%
11	12.651	1793	1796	1802	rBV	179770	145647	2.24%	0.336%
12	12.827	1821	1826	1829	rBV	6012620	5913514	90.85%	13.648%
13	13.357	1913	1916	1920	rBV	121594	97659	1.50%	0.225%
14	13.874	2000	2004	2024	rBV	1330401	1351632	20.76%	3.119%
15	14.651	2131	2136	2141	rBV	94497	110800	1.70%	0.256%
16	14.968	2186	2190	2199	rBV	114328	137252	2.11%	0.317%
17	15.292	2240	2245	2249	rBV	858092	1081094	16.61%	2.495%
18	15.327	2249	2251	2262	rVB	146992	210188	3.23%	0.485%
19	15.739	2317	2321	2329	rBV	100759	153956	2.37%	0.355%
20	16.215	2397	2402	2412	rBV	84581	149748	2.30%	0.346%
21	16.362	2415	2427	2440	rBV5	39217	179932	2.76%	0.415%
22	16.774	2491	2497	2507	rVB3	49611	106953	1.64%	0.247%
23	17.433	2604	2609	2617	rVB3	30453	74265	1.14%	0.171%

Sum of corrected areas: 43328891

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Misc :
ALS Vial : 3 Sample Multiplier: 1

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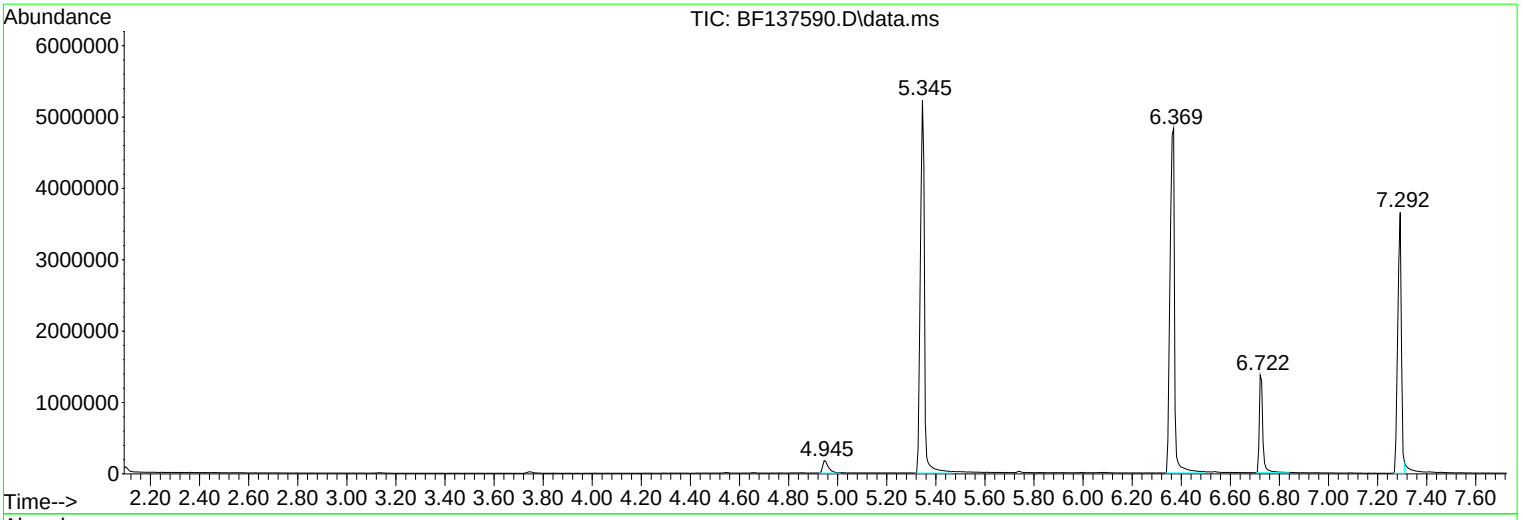
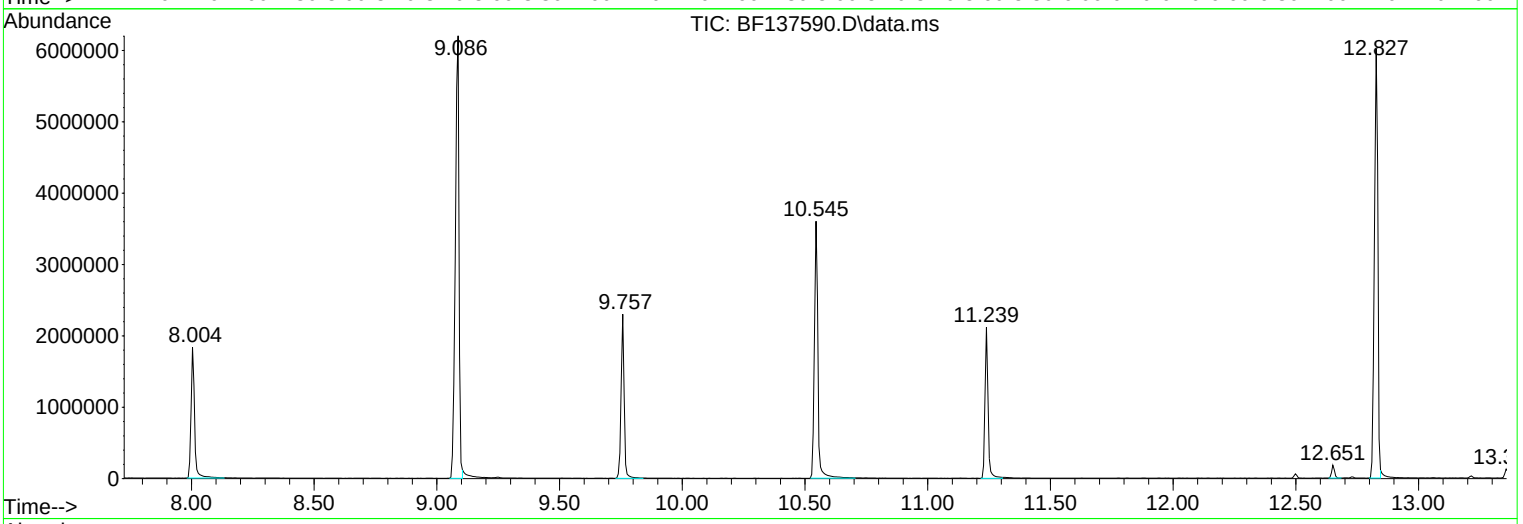
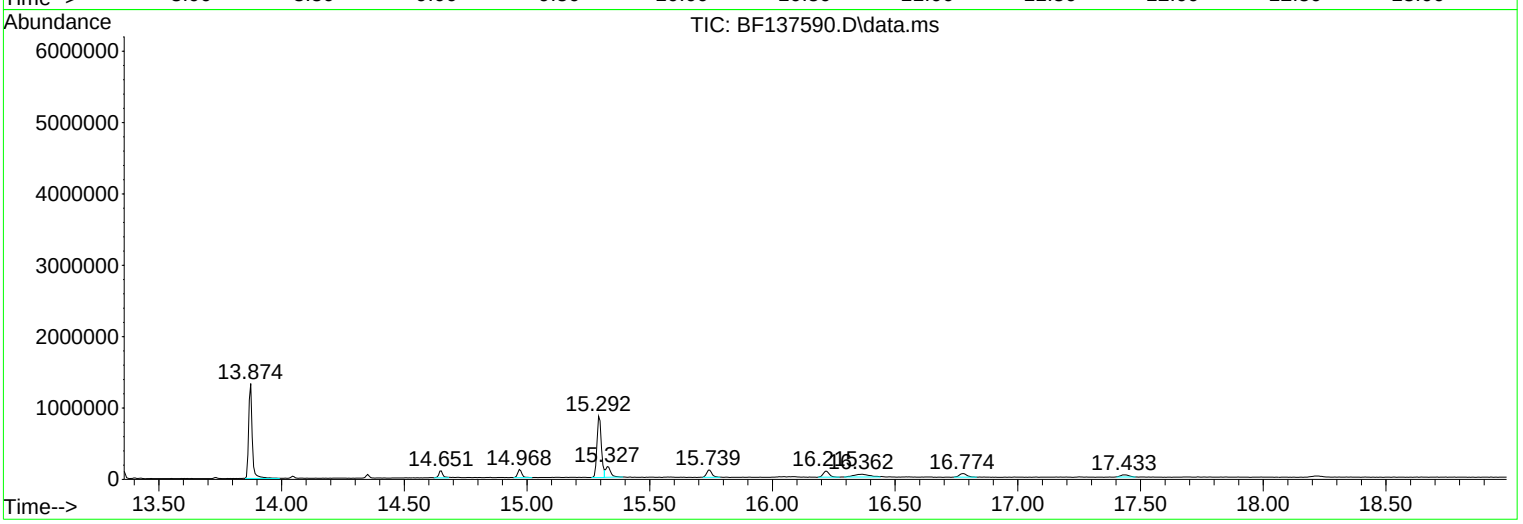
ClientSampleId :
PB159568BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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

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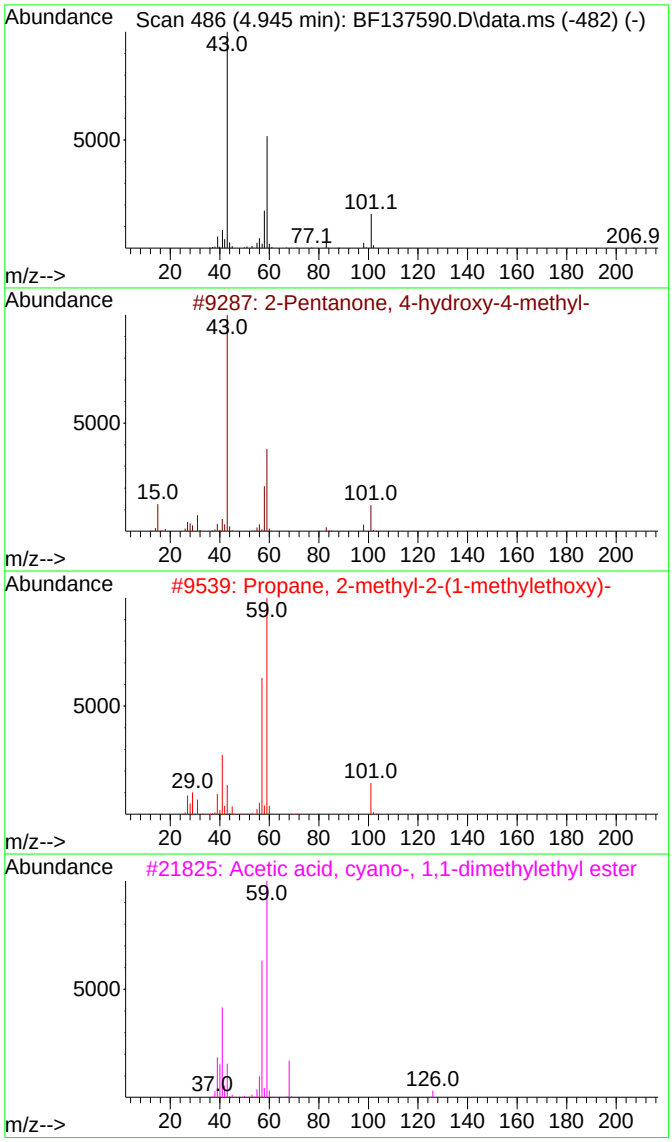
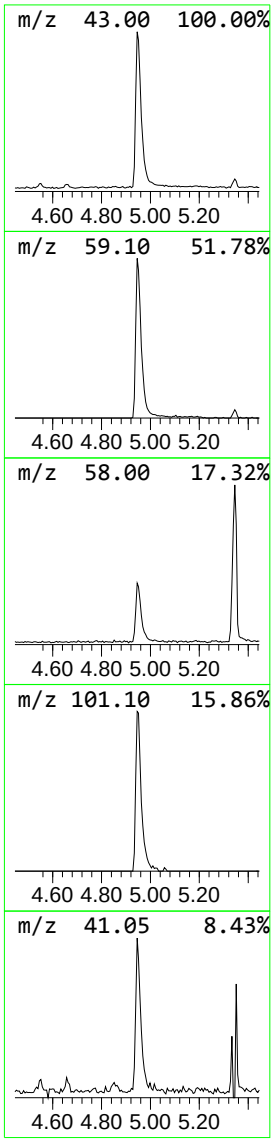
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.945	4.18 ng	285898	1,4-Dichlorobenzene-d4	6.728

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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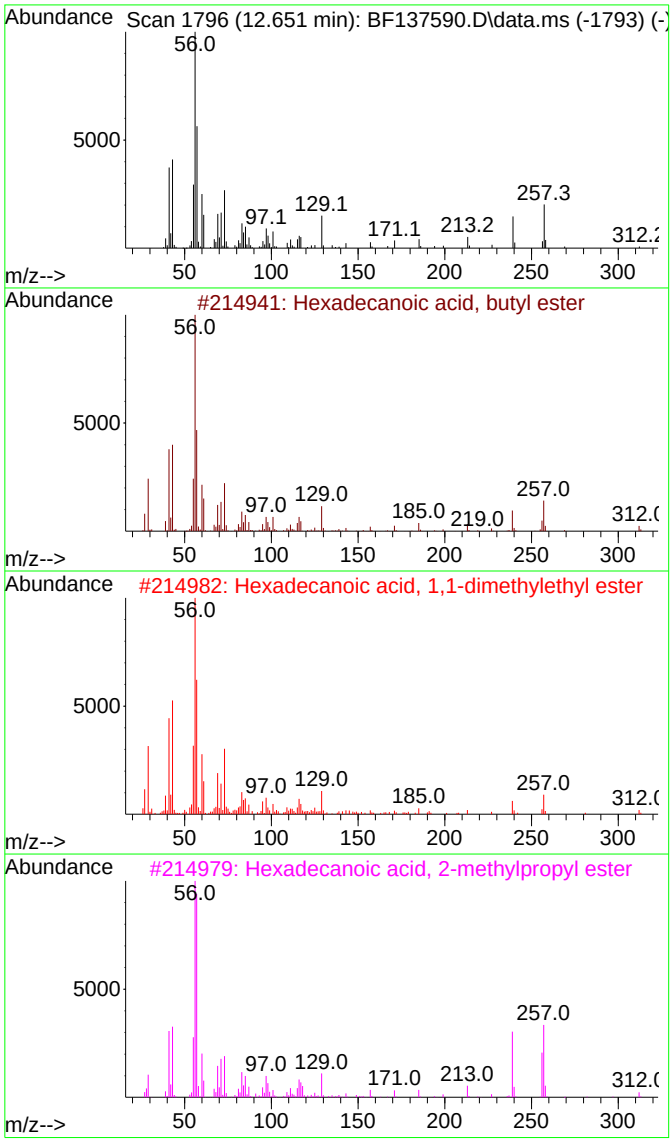
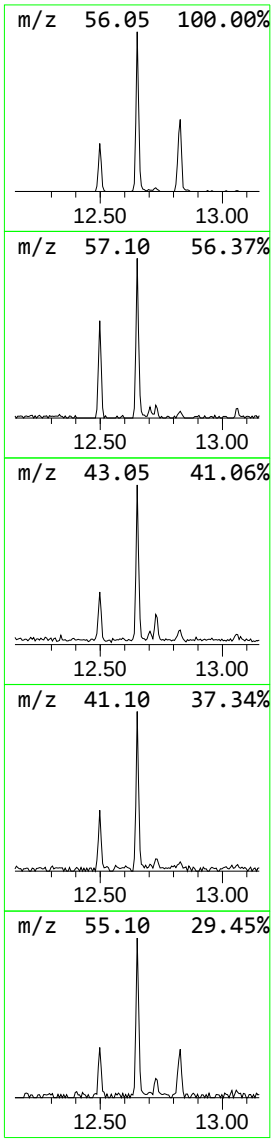
****
Peak Number 2 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.651	2.16 ng	145647	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	46
4	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	37
5	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35





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Instrument :
BNA_F
ClientSampleId :
PB159568BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
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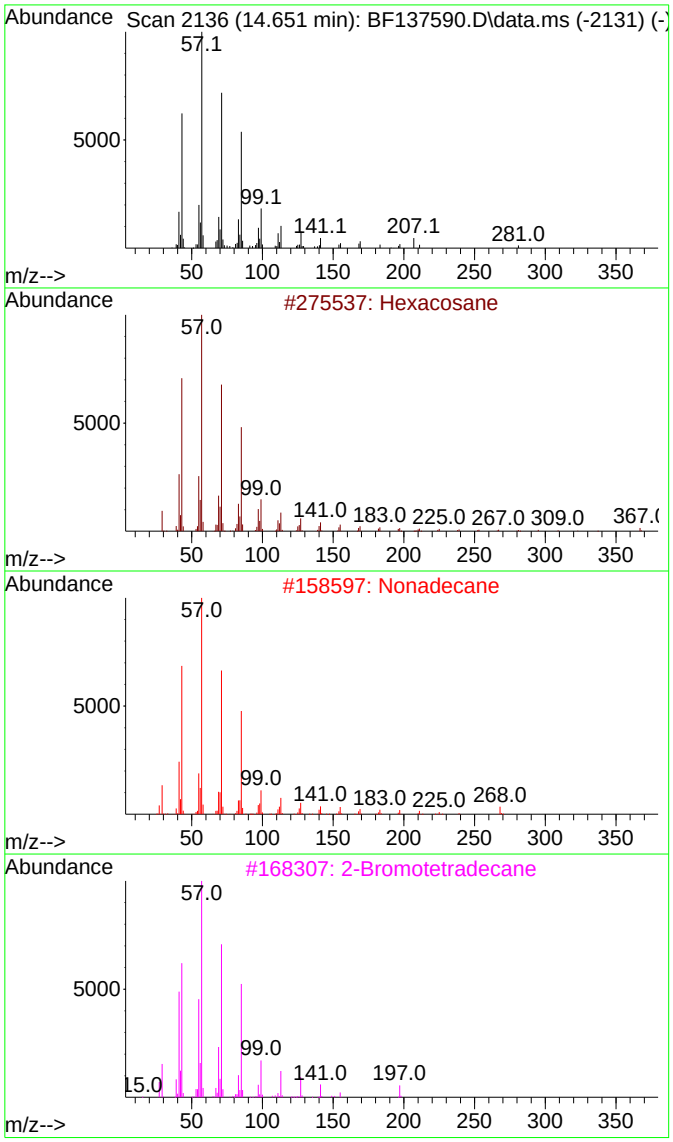
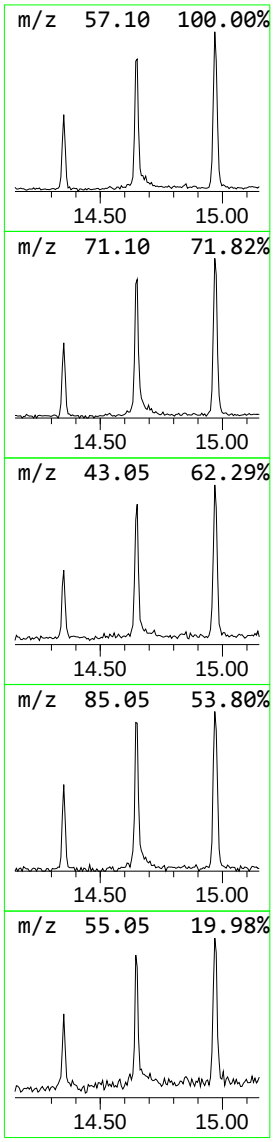
Peak Number 3 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.651	2.05 ng	110800	Perylene-d12	15.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Nonadecane	268	C19H40	000629-92-5	87
3	2-Bromotetradecane	276	C14H29Br	074036-95-6	87
4	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86





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BNA_F
ClientSampleId :
PB159568BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
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TIC Library : C:\Database\NIST20.L
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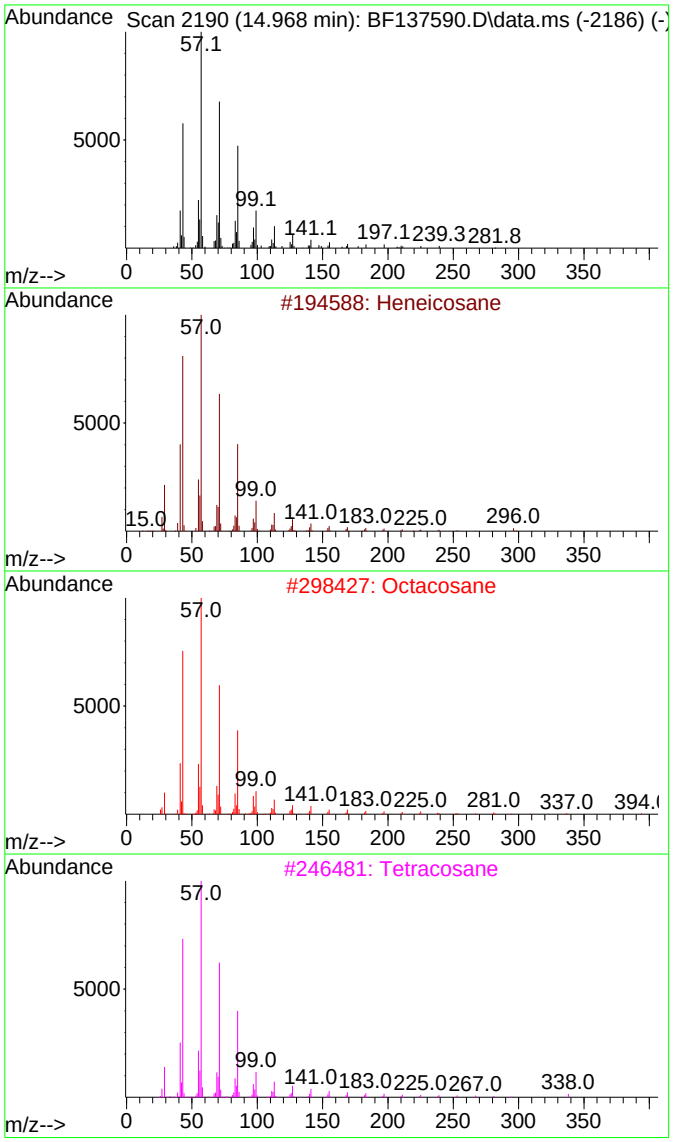
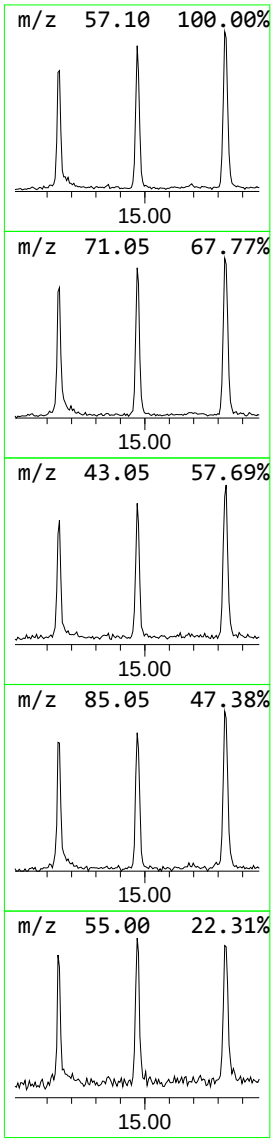
Peak Number 4 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.968	2.54 ng	137252	Perylene-d12	15.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5	Pentacosane	352	C25H52	000629-99-2	90





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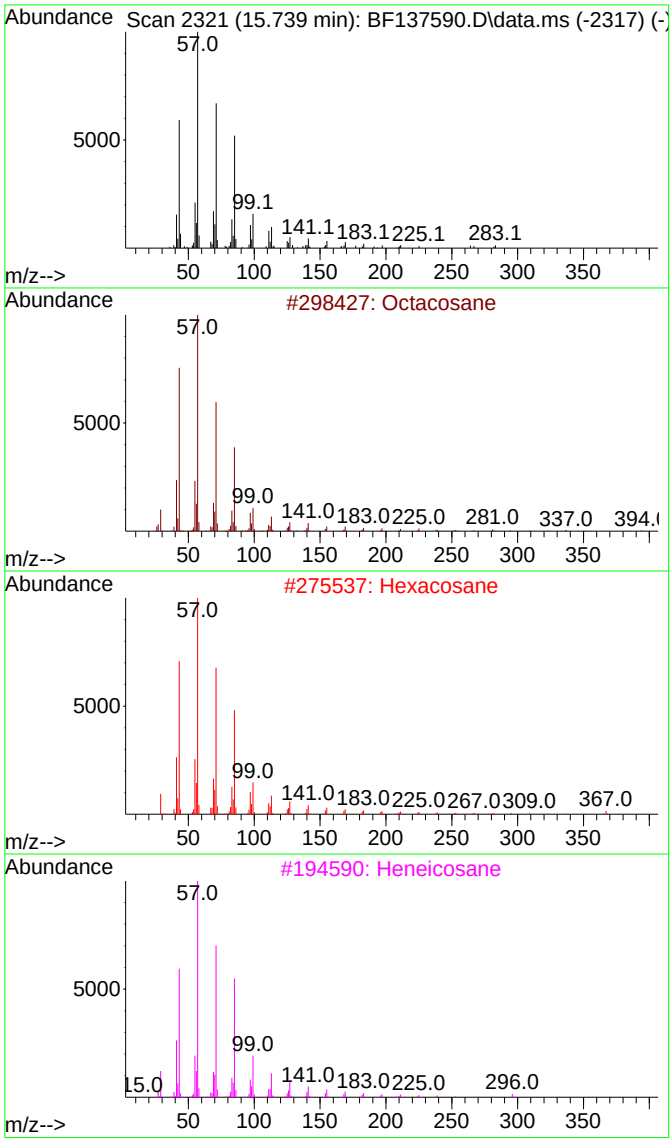
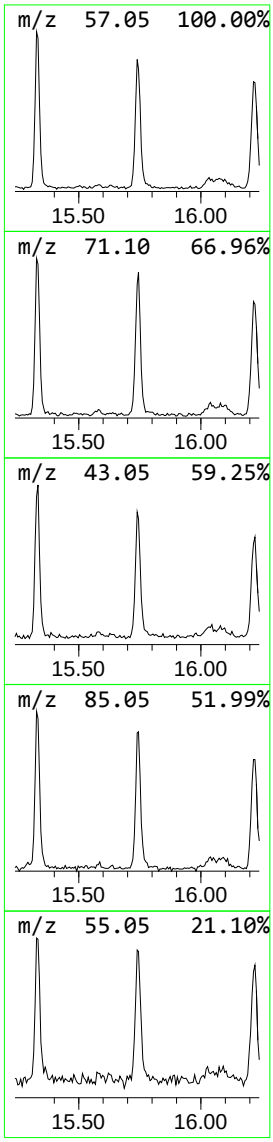
****

Peak Number 5 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.739	2.85 ng	153956	Perylene-d12	15.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Tetratetracontane	619	C44H90	007098-22-8	87
5	Heptadecane	240	C17H36	000629-78-7	87





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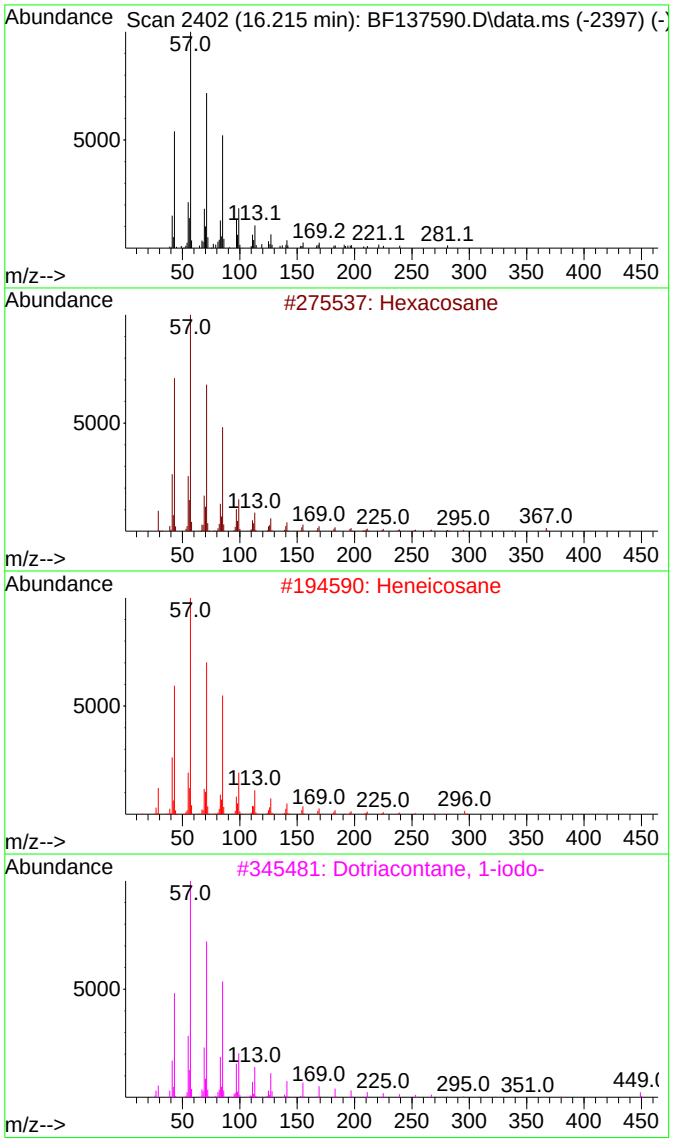
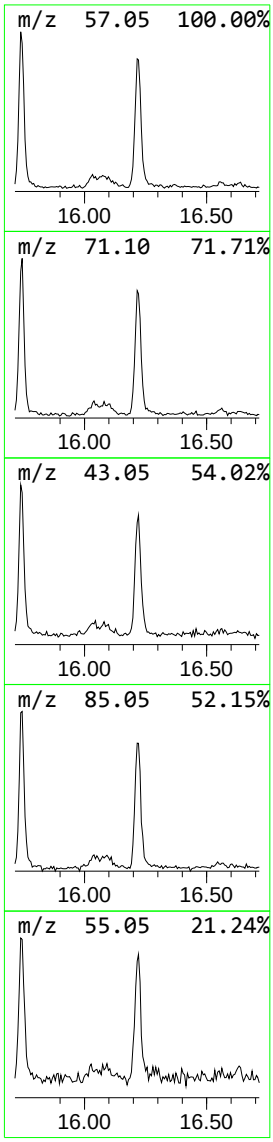
****

Peak Number 6 Dotriacontane, 1-iodo- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.215	2.77 ng	149748	Perylene-d12	15.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	87
3	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	86
4	2-Bromotetradecane	276	C14H29Br	074036-95-6	86
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	86





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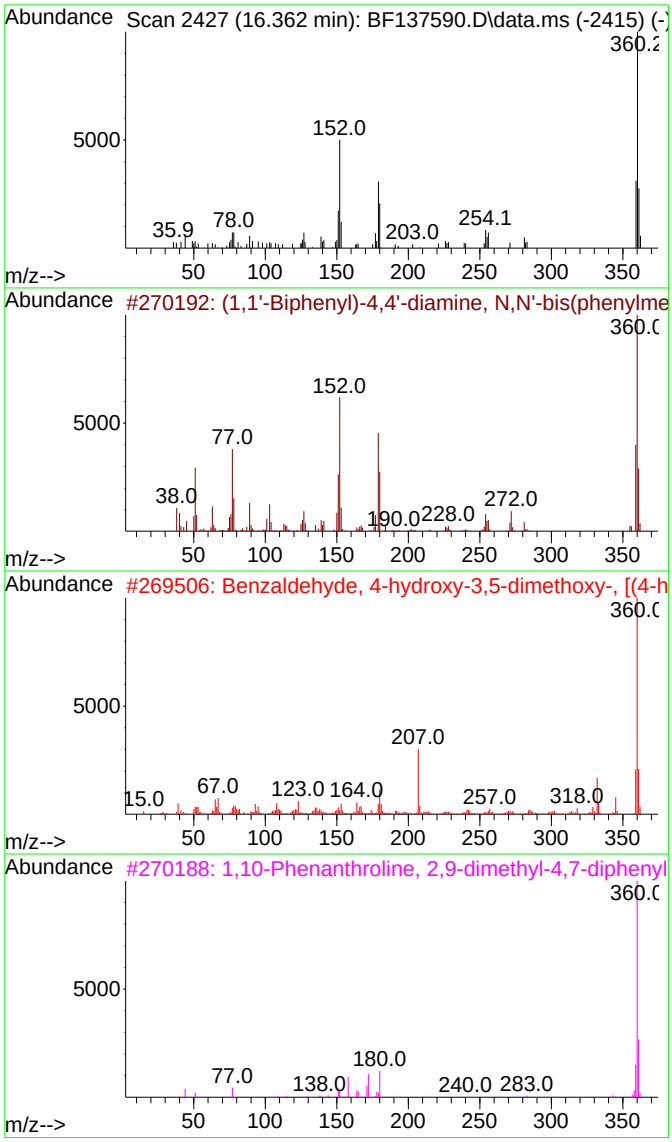
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

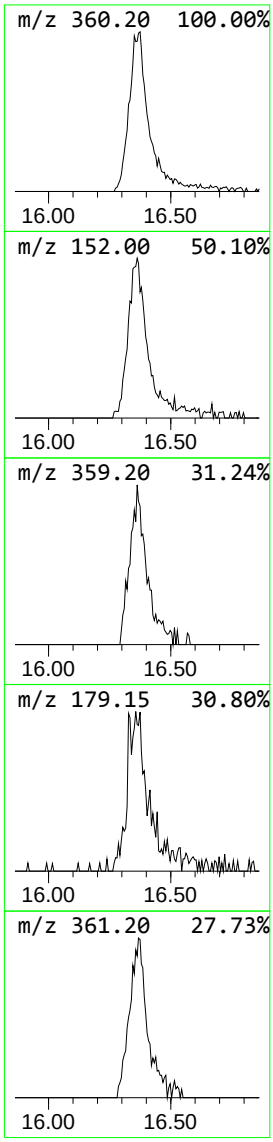
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.362	3.33 ng	179932	Perylene-d12	15.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1,1'-Biphenyl)-4,4'-diamine, N,...	360	C26H20N2	006311-48-4	94
2	Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	47
3	1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	47
4	Jaceidin	360	C18H16O8	010173-01-0	43
5	1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13BO6	1000150-23-7	43





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.945	4.2	ng	285898	1	6.728	1368380	20.0
Hexadecanoic ac...	12.651	2.2	ng	145647	5	13.874	1351630	20.0
Hexacosane	14.651	2.0	ng	110800	6	15.292	1081090	20.0
Heneicosane	14.968	2.5	ng	137252	6	15.292	1081090	20.0
Octacosane	15.739	2.9	ng	153956	6	15.292	1081090	20.0
Dotriacontane, ...	16.215	2.8	ng	149748	6	15.292	1081090	20.0
(1,1'-Biphenyl)...	16.362	3.3	ng	179932	6	15.292	1081090	20.0