LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130966.D
Acq On : 03 Nov 2022 18:42
Operator : CG\JU
Sample : PB148686BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148686BL

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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130966.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.269	23	31	38	rVB	124432	179852	4.92%	0.807%
2	2.381	45	50	56	rVB	53292	69090	1.89%	0.310%
3	5.157	517	522	537	rVB	335221	444698	12.16%	1.995%
4	5.540	582	587	590	rBV	2684163	2863498	78.33%	12.848%
5	6.539	751	757	760	rBV	2693192	2874383	78.63%	12.897%
6	6.916	817	821	824	rBV	749719	598059	16.36%	2.683%
7	7.481	911	917	920	rBV	1854426	1896320	51.87%	8.508%
8	8.198	1034	1039	1043	rBV	804208	782277	21.40%	3.510%
9	9.280	1217	1223	1226	rBV	3585371	3371986	92.24%	15.129%
10	9.963	1333	1339	1342	rBV	1026909	863122	23.61%	3.873%
11	10.757	1468	1474	1477	rBV	2085893	1971171	53.92%	8.844%
12	11.457	1589	1593	1596	rBV	1135444	998408	27.31%	4.480%
13	13.051	1858	1864	1867	rBV	3524963	3655601	100.00%	16.402%
14	14.104	2039	2043	2046	rBV	846793	740074	20.24%	3.321%
15	14.198	2053	2059	2064	rBV	44602	58817	1.61%	0.264%
16	14.880	2171	2175	2180	rBV	36069	41032	1.12%	0.184%
17	15.233	2232	2235	2239	rBV	35793	41748	1.14%	0.187%
18	15.609	2293	2299	2311	rBV	416818	588919	16.11%	2.642%
19	16.086	2374	2380	2387	rBV2	44472	81996	2.24%	0.368%
20	16.621	2466	2471	2480	rVB2	32837	59184	1.62%	0.266%
21	17.509	2615	2622	2626	rBV5	23172	59569	1.63%	0.267%
22	17.986	2698	2703	2712	rVB3	19207	47847	1.31%	0.215%

Sum of corrected areas: 22287651

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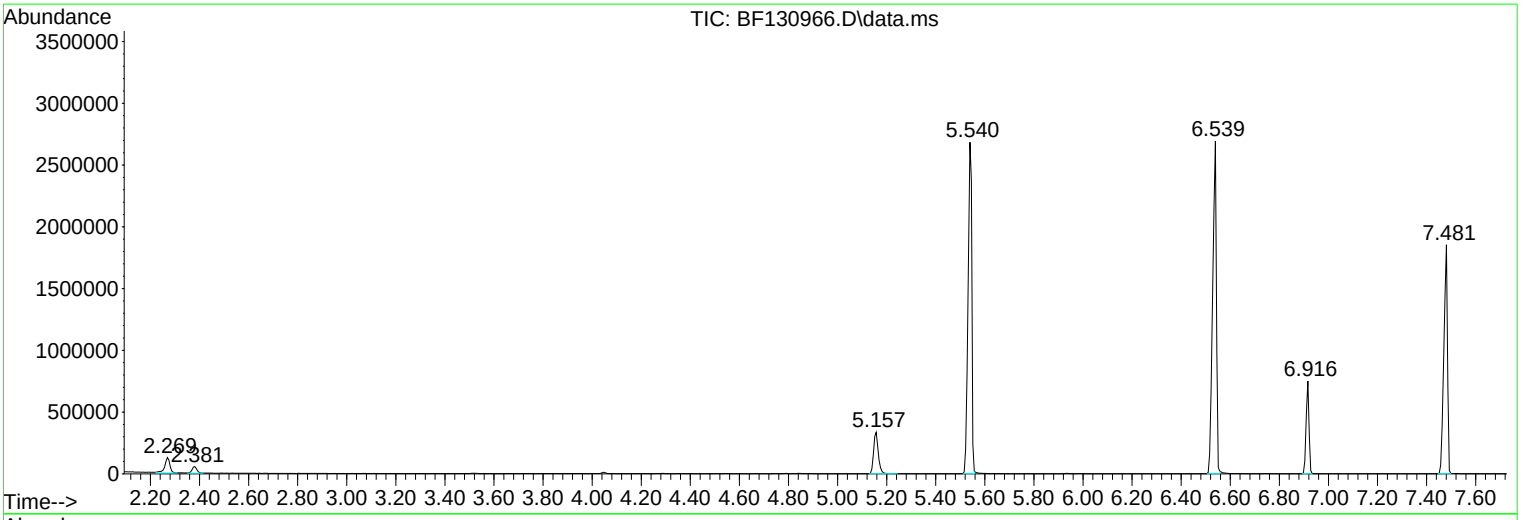
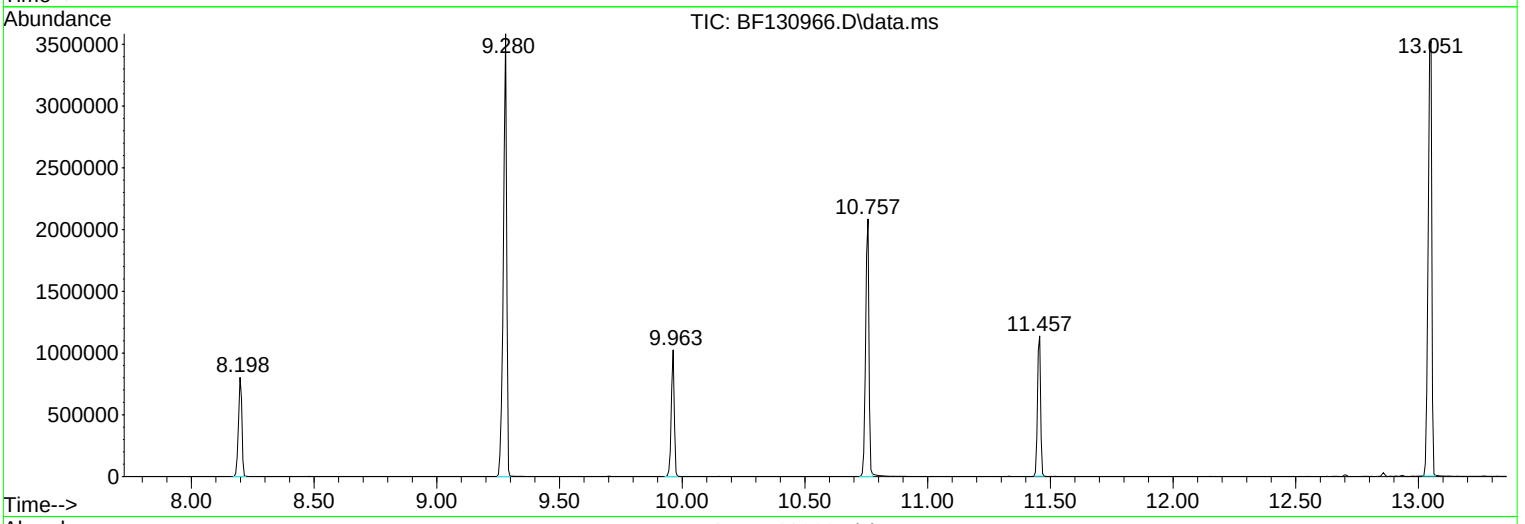
ALS Vial : 3 Sample Multiplier: 1

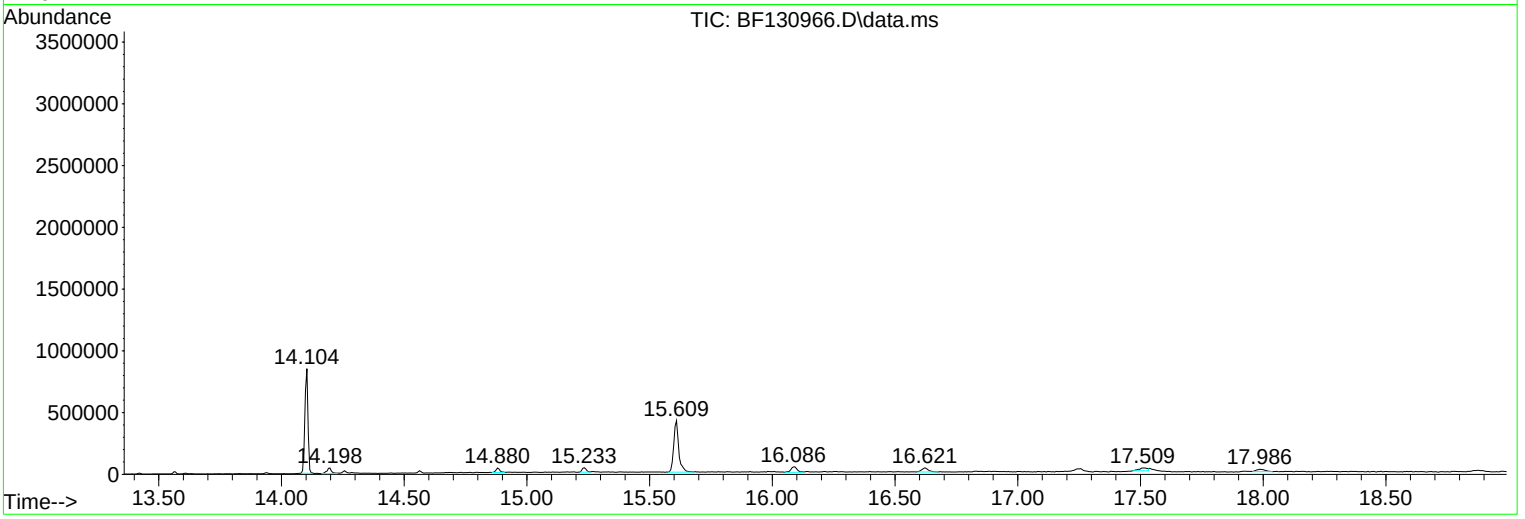
Instrument :
BNA_F
ClientSampleId :
PB148686BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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

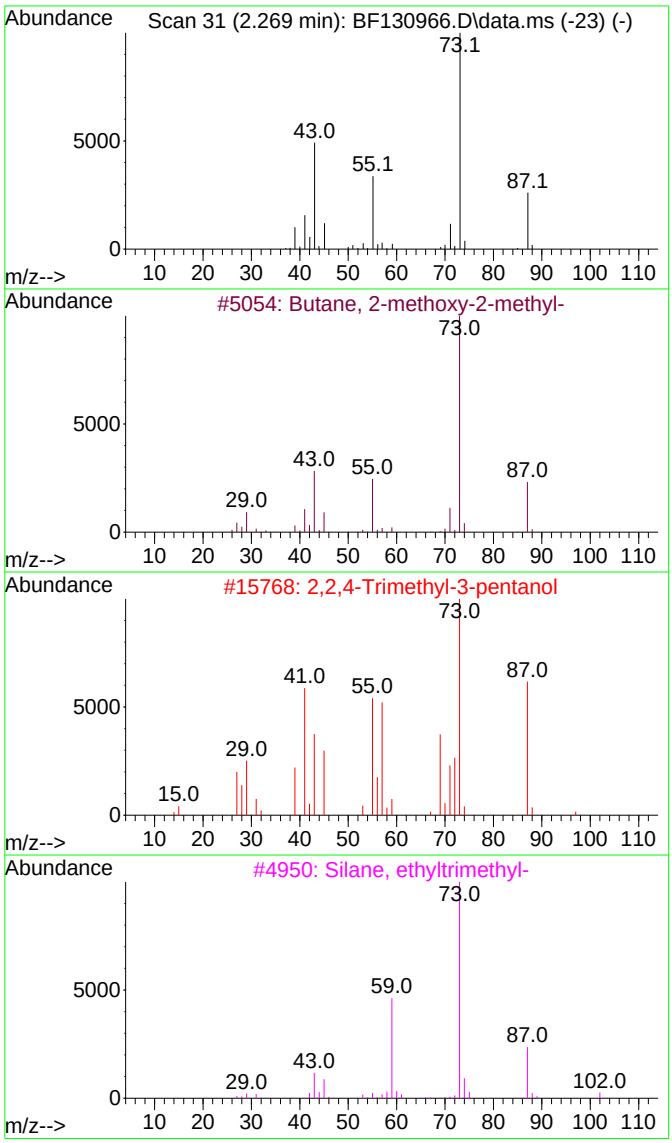
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

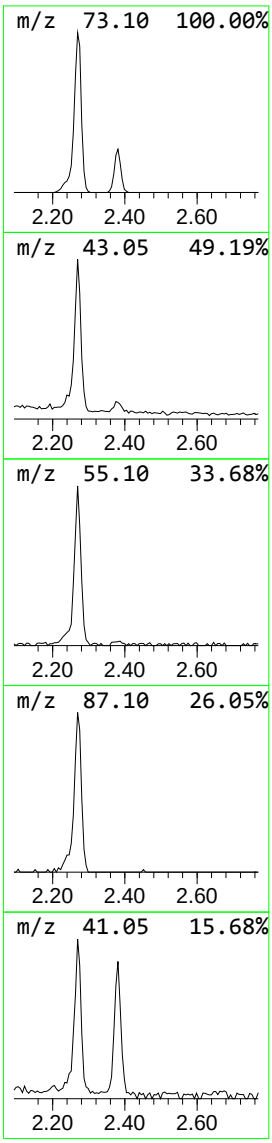
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.269	6.01 ng	179852	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25





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TIC Library : C:\Database\NIST20.L
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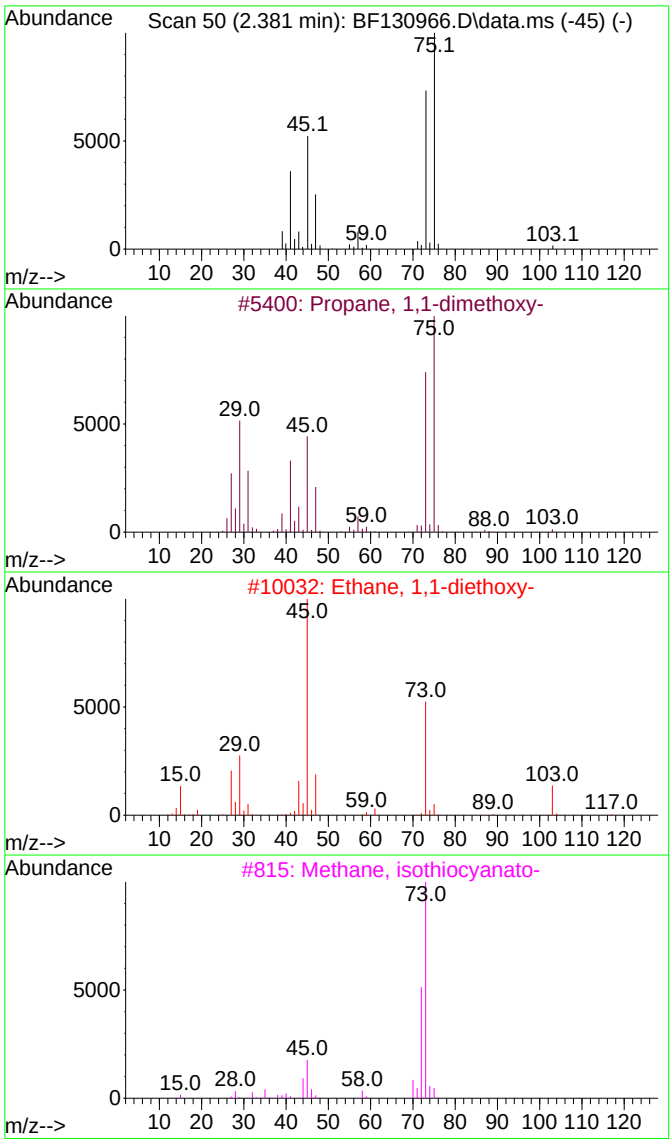
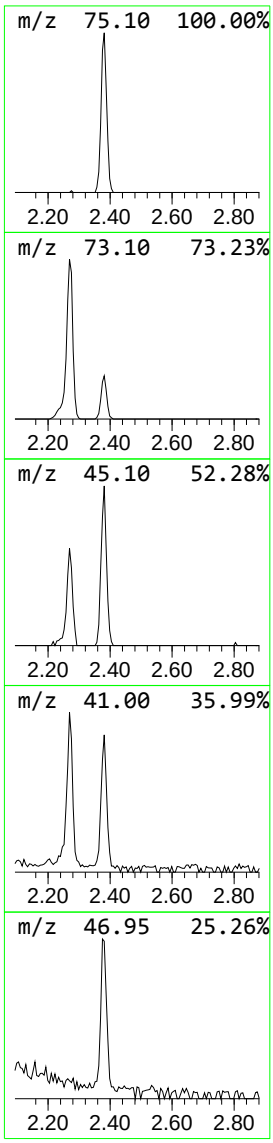
Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.381	2.31 ng	69090	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2	Ethane, 1,1-diethoxy-	118	C6H14O2	000105-57-7	17
3	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
4	3-Hexene, 1-(1-ethoxyethoxy)-, (Z)-	172	C10H20O2	028069-74-1	9
5	2-Hexanol, 5-methyl-	116	C7H16O	000627-59-8	9





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Operator : CG\JU
Sample : PB148686BL
Misc :
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Instrument :
BNA_F
ClientSampleId :
PB148686BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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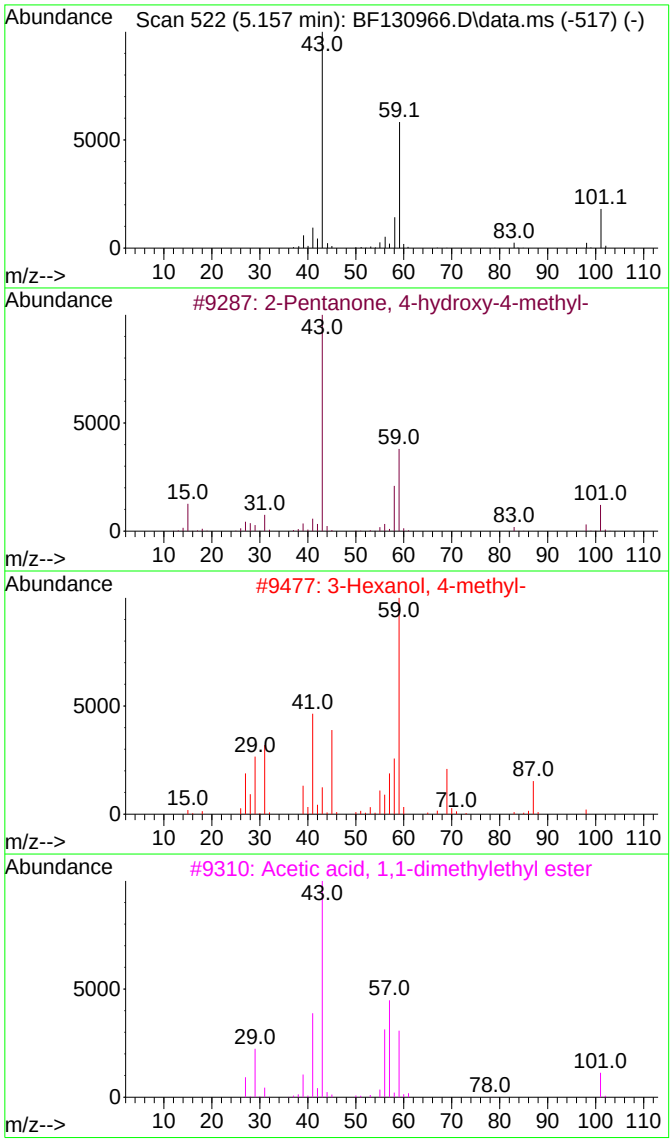
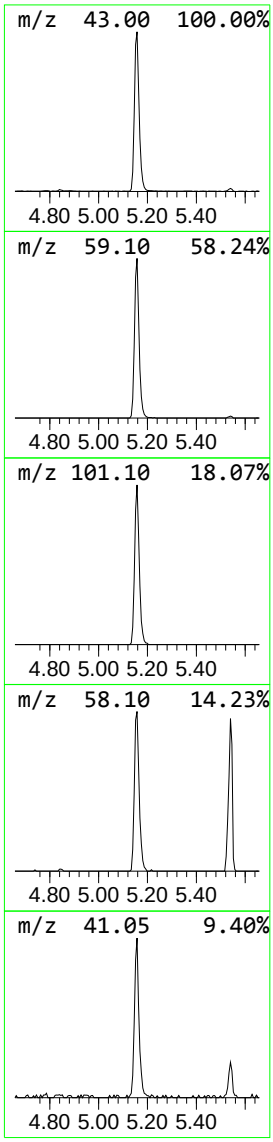
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.157	14.87 ng	444698	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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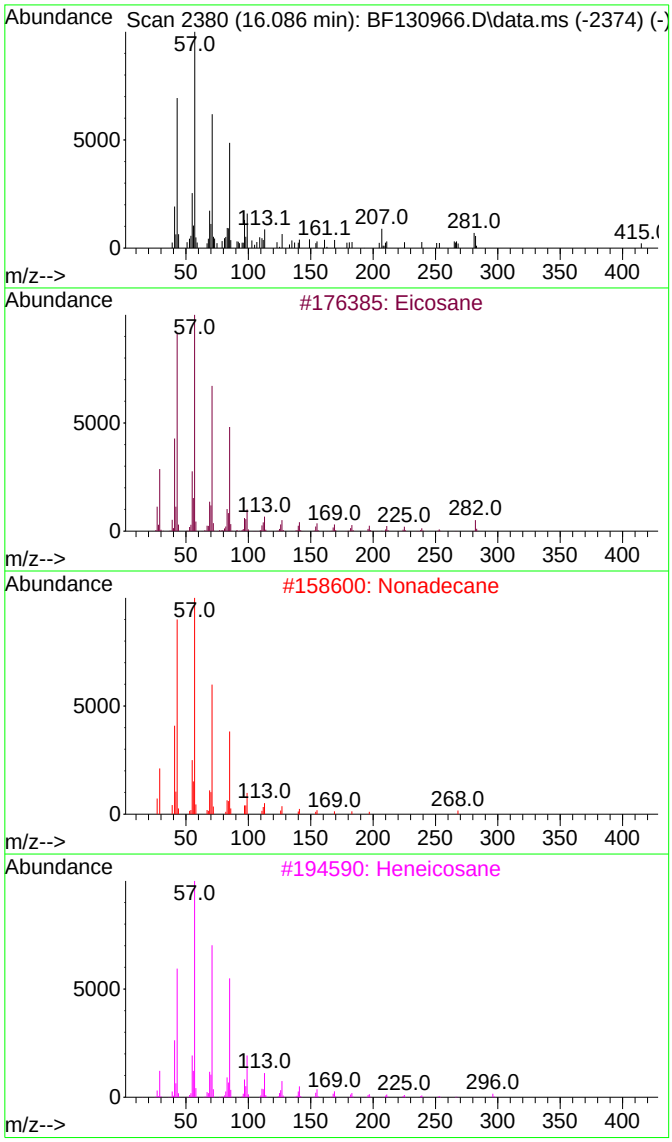
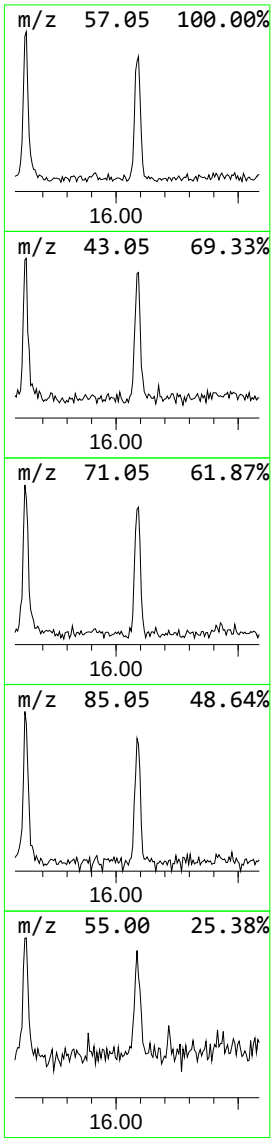
Peak Number 4 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.086	2.78 ng	81996	Perylene-d12	15.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Nonadecane	268	C19H40	000629-92-5	94
3	Heneicosane	296	C21H44	000629-94-7	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Pentacosane	352	C25H52	000629-99-2	90





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Operator : CG\JU
Sample : PB148686BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148686BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
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TIC Library : C:\Database\NIST20.L
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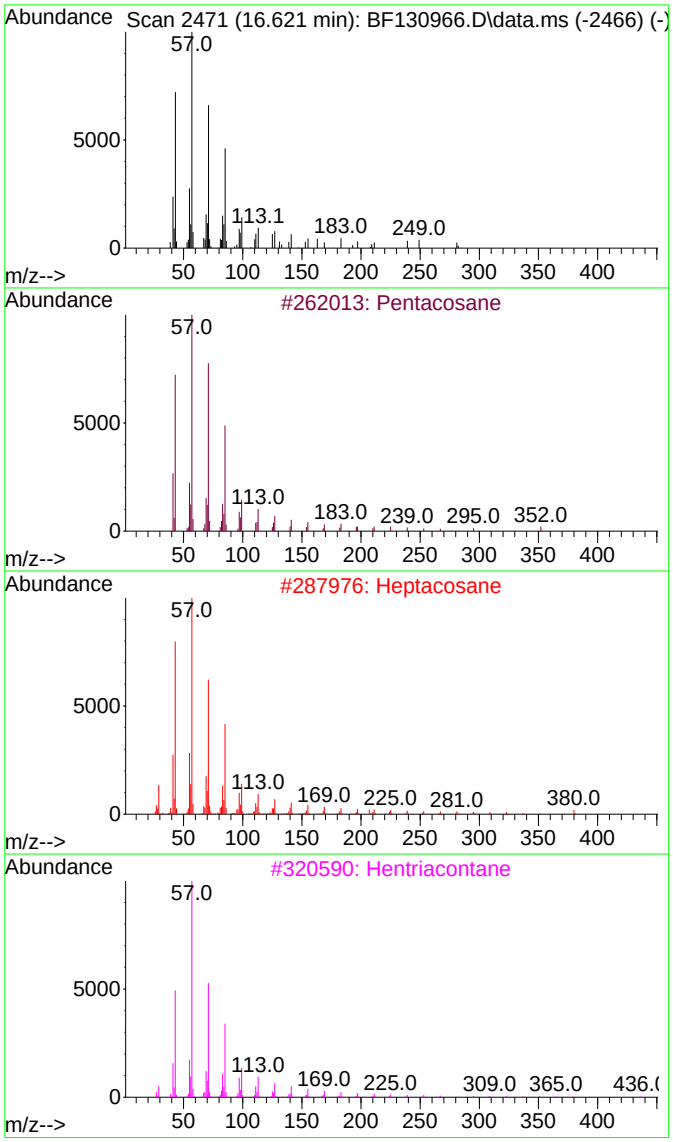
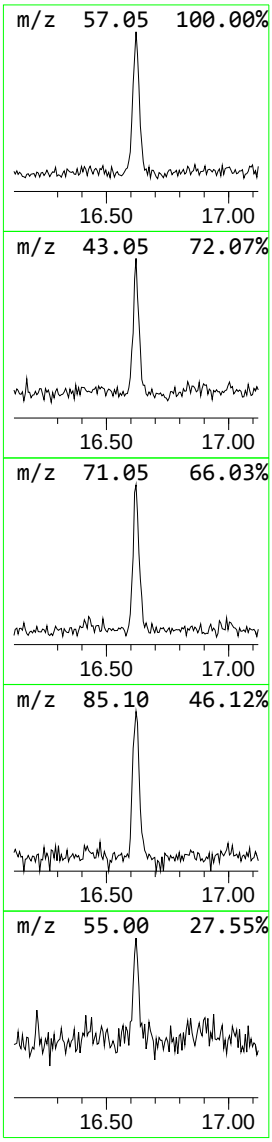
Peak Number 5 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.621	2.01 ng	59184	Perylene-d12	15.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	90
2	Heptacosane	380	C27H56	000593-49-7	90
3	Hentriacontane	437	C31H64	000630-04-6	87
4	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	87
5	Octadecane	254	C18H38	000593-45-3	87





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Sample : PB148686BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

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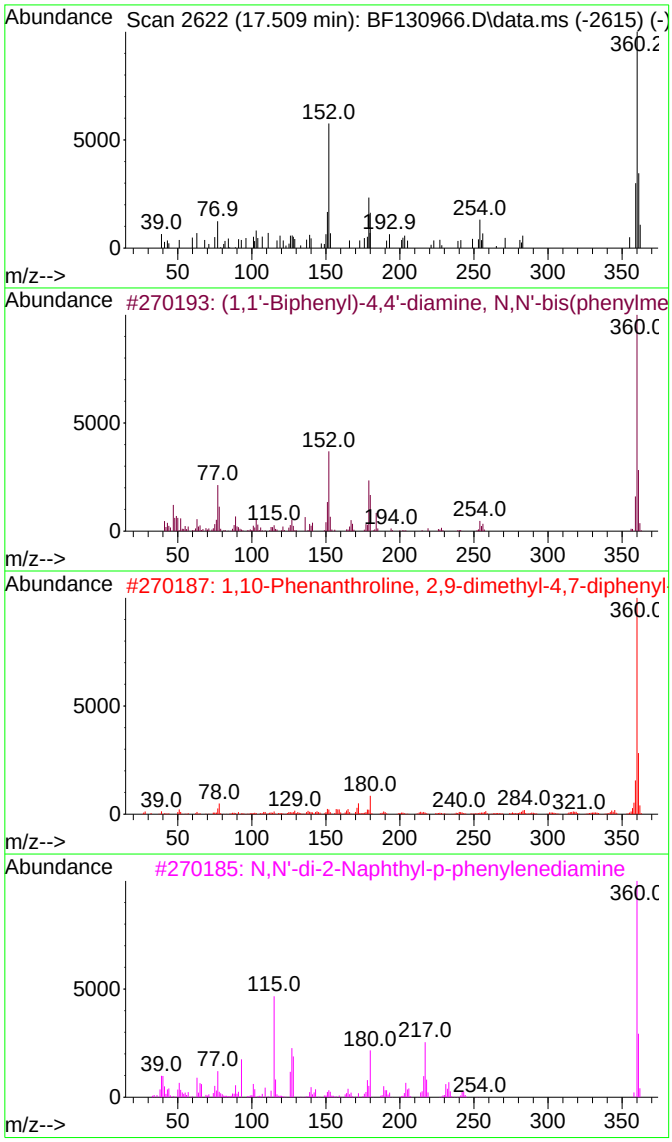
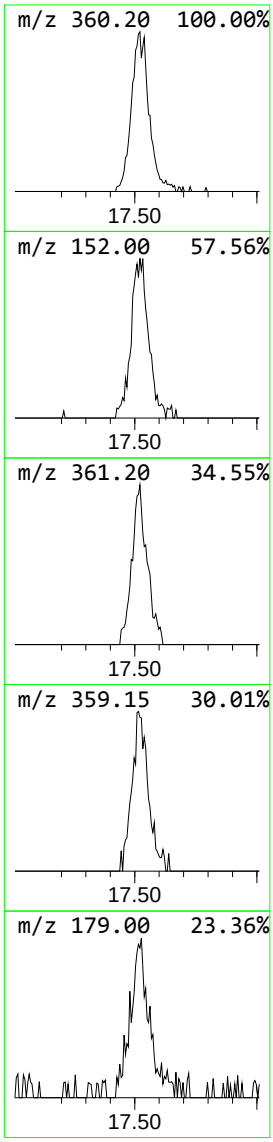
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.509	2.02 ng	59569	Perylene-d12	15.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1,1'-Biphenyl)-4,4'-diamine, N,...	360	C26H20N2	006311-48-4	68
2	1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	47
3	N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	43
4	Benzoic acid, 4-(3,4-dihydro-2,4...	361	C20H15N3O4	317326-96-8	35
5	3-Amino-6-nitro-4-phenylsulfanyl...	360	C16H12N2O4S2	1000275-36-3	35





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
Butane, 2-metho...	2.269	6.0	ng	179852	1	6.916	598059	20.0
Propane, 1,1-di...	2.381	2.3	ng	69090	1	6.916	598059	20.0
2-Pentanone, 4-...	5.157	14.9	ng	444698	1	6.916	598059	20.0
Eicosane	16.086	2.8	ng	81996	6	15.610	588919	20.0
Pentacosane	16.621	2.0	ng	59184	6	15.610	588919	20.0
(1,1'-Biphenyl)...	17.509	2.0	ng	59569	6	15.610	588919	20.0