LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
Data File : BF106460.D
Acq On : 14 Jun 2018 23:18
Operator : JU/SJ
Sample : J3471-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : #2

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-BF061118.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.201	483	487	496	rVB	200840	217233	6.85%	0.788%
2	5.613	553	557	564	rBV	2217020	2311139	72.90%	8.378%
3	6.613	723	727	734	rBV	2267907	2300033	72.55%	8.338%
4	6.748	746	750	753	rBV	2637663	2263538	71.40%	8.206%
5	6.966	783	787	790	rBV	979172	749089	23.63%	2.716%
6	7.125	809	814	817	rBV	2046040	1820540	57.42%	6.600%
7	7.531	878	883	886	rBV	1502000	1493218	47.10%	5.413%
8	8.248	1001	1005	1008	rBV	1144359	906144	28.58%	3.285%
9	9.319	1181	1187	1191	rBV	2415389	2311863	72.92%	8.381%
10	9.713	1250	1254	1259	rVB	261965	205049	6.47%	0.743%
11	9.919	1285	1289	1294	rBV2	44707	52247	1.65%	0.189%
12	10.007	1298	1304	1317	rVB2	1046206	952114	30.03%	3.452%
13	10.419	1372	1374	1377	rVB2	58704	48072	1.52%	0.174%
14	10.801	1435	1439	1442	rBV	1408323	1272968	40.15%	4.615%
15	10.895	1452	1455	1461	rBV2	54261	73826	2.33%	0.268%
16	11.342	1528	1531	1534	rBV	39701	36209	1.14%	0.131%
17	11.501	1554	1558	1560	rBV	871725	835881	26.36%	3.030%
18	11.519	1560	1561	1568	rVV	161846	141611	4.47%	0.513%
19	12.001	1640	1643	1645	rBV2	33374	37034	1.17%	0.134%
20	12.113	1658	1662	1664	rBV2	44495	47804	1.51%	0.173%
21	12.177	1670	1673	1676	rBV3	31170	31863	1.01%	0.116%
22	12.442	1713	1718	1722	rBV3	51810	58841	1.86%	0.213%
23	12.713	1761	1764	1767	rBV	396719	325043	10.25%	1.178%
24	12.748	1767	1770	1773	rVB	186376	153930	4.86%	0.558%
25	12.871	1788	1791	1793	rBV2	36836	36544	1.15%	0.132%
26	12.942	1797	1803	1809	rBV	344567	406319	12.82%	1.473%
27	13.083	1823	1827	1830	rBV	2224679	1931201	60.91%	7.001%
28	13.218	1848	1850	1853	rBV	53721	41397	1.31%	0.150%
29	13.271	1856	1859	1861	rVV2	61912	57808	1.82%	0.210%
30	13.336	1868	1870	1872	rVB	40719	34745	1.10%	0.126%
31	13.448	1887	1889	1891	rVB	39965	31837	1.00%	0.115%
32	13.542	1903	1905	1908	rVB3	46601	42908	1.35%	0.156%
33	13.965	1974	1977	1983	rBV3	241026	281180	8.87%	1.019%
34	14.148	2003	2008	2011	rBV2	866271	919433	29.00%	3.333%

LSC Area Percent Report

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Data File : BF106460.D
Acq On : 14 Jun 2018 23:18
Operator : JU/SJ
Sample : J3471-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : #2

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-BF061118.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.171	2011	2012	2015	rVB	141485	86520	2.73%	0.314%
36	14.289	2020	2032	2050	rBV7	683200	3170426	100.00%	11.493%
37	14.612	2083	2087	2094	rBV2	240637	380767	12.01%	1.380%
38	15.083	2164	2167	2172	rVB	107798	118392	3.73%	0.429%
39	15.224	2189	2191	2195	rBV	103140	158589	5.00%	0.575%
40	15.283	2198	2201	2204	rVB	387115	390180	12.31%	1.414%
41	15.683	2265	2269	2274	rVB	420716	517227	16.31%	1.875%
42	15.906	2304	2307	2312	rBV4	112652	147512	4.65%	0.535%
43	16.148	2345	2348	2353	rVB	122428	186364	5.88%	0.676%

Sum of corrected areas: 27584638

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
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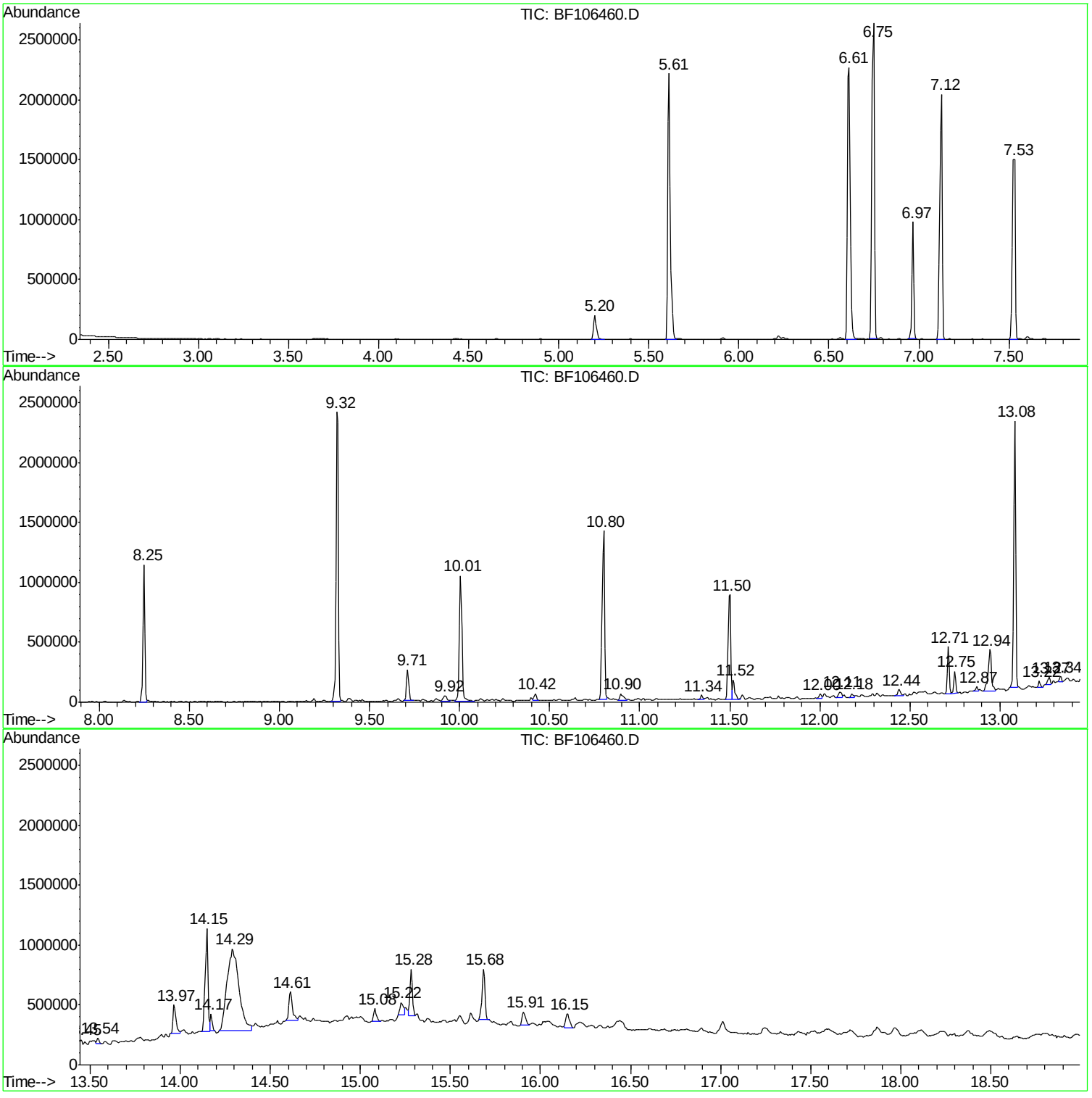
Instrument : BNA_F
ClientSampleId : #2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
Data File : BF106460.D
Acq On : 14 Jun 2018 23:18
Operator : JU/SJ
Sample : J3471-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : #2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

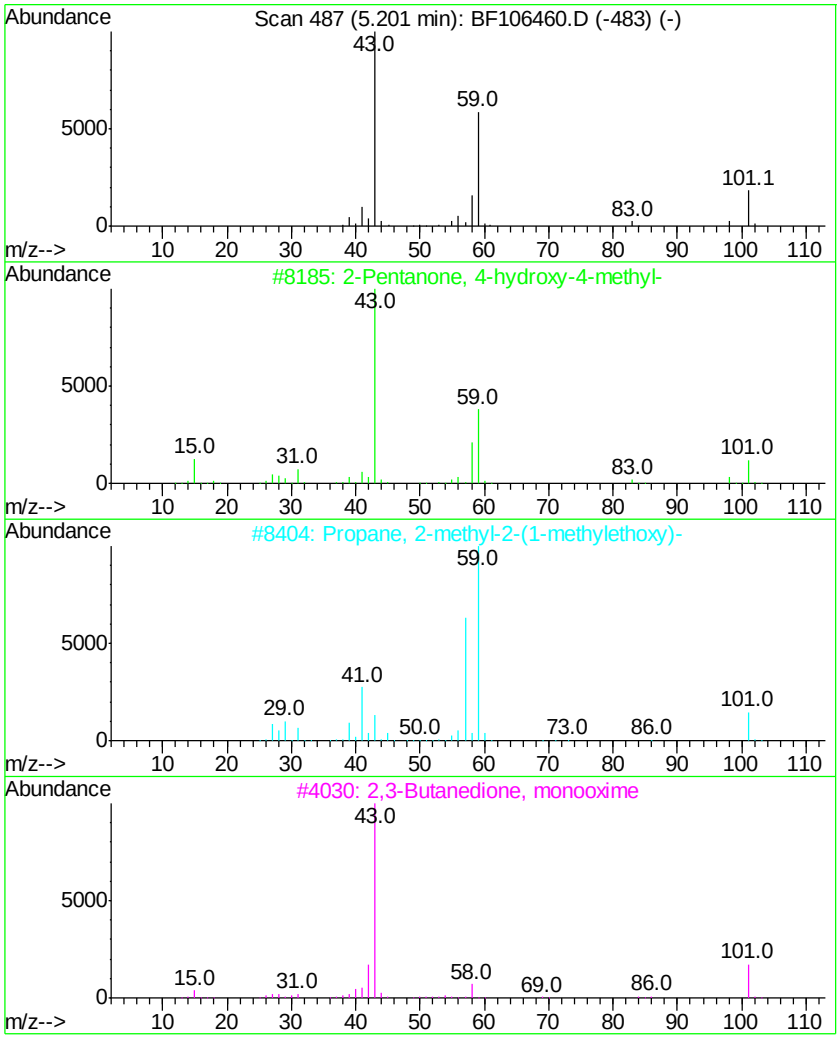
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

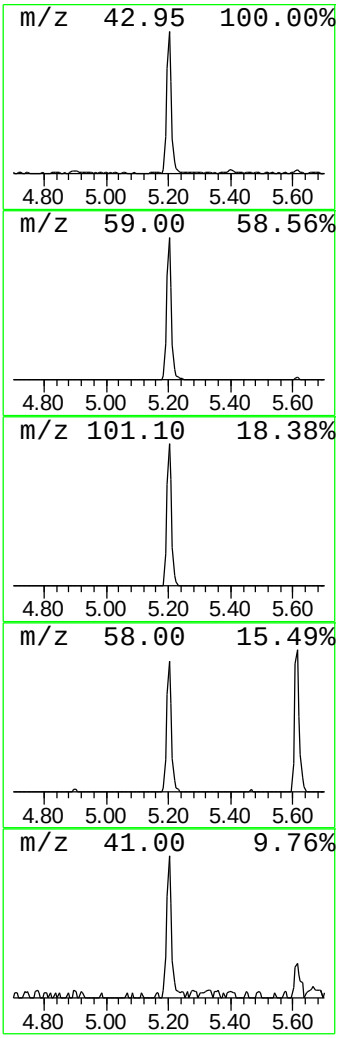
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	5.80 ng	217233	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	3-Octanol	130	C8H18O	000589-98-0	9





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Data File : BF106460.D
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Sample : J3471-04
Misc :
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Instrument : BNA_F
ClientSampleId : #2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

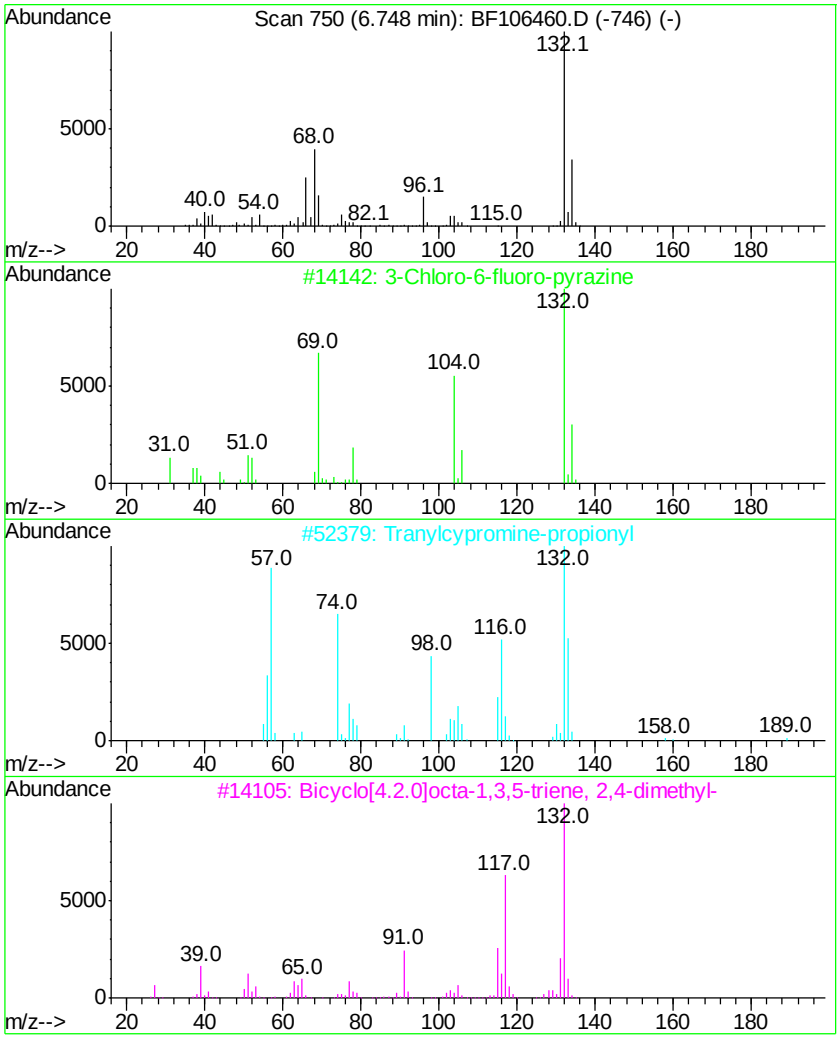
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

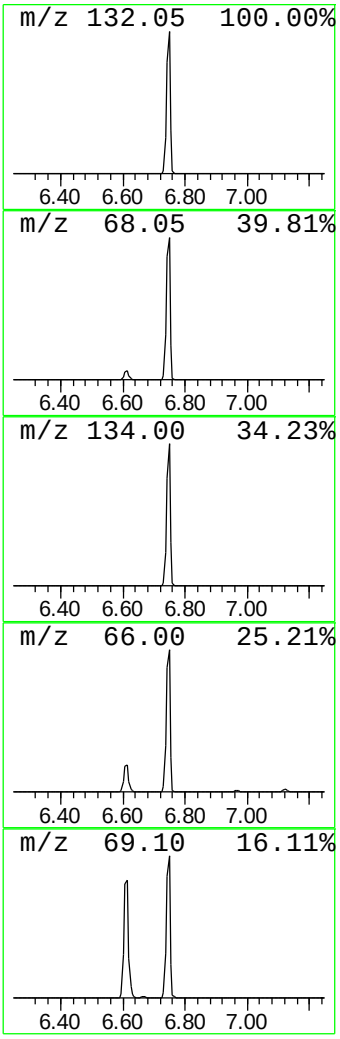
****

Peak Number 2 unknown6.75 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	60.43 ng	2263540	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
Data File : BF106460.D
Acq On : 14 Jun 2018 23:18
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Sample : J3471-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : #2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

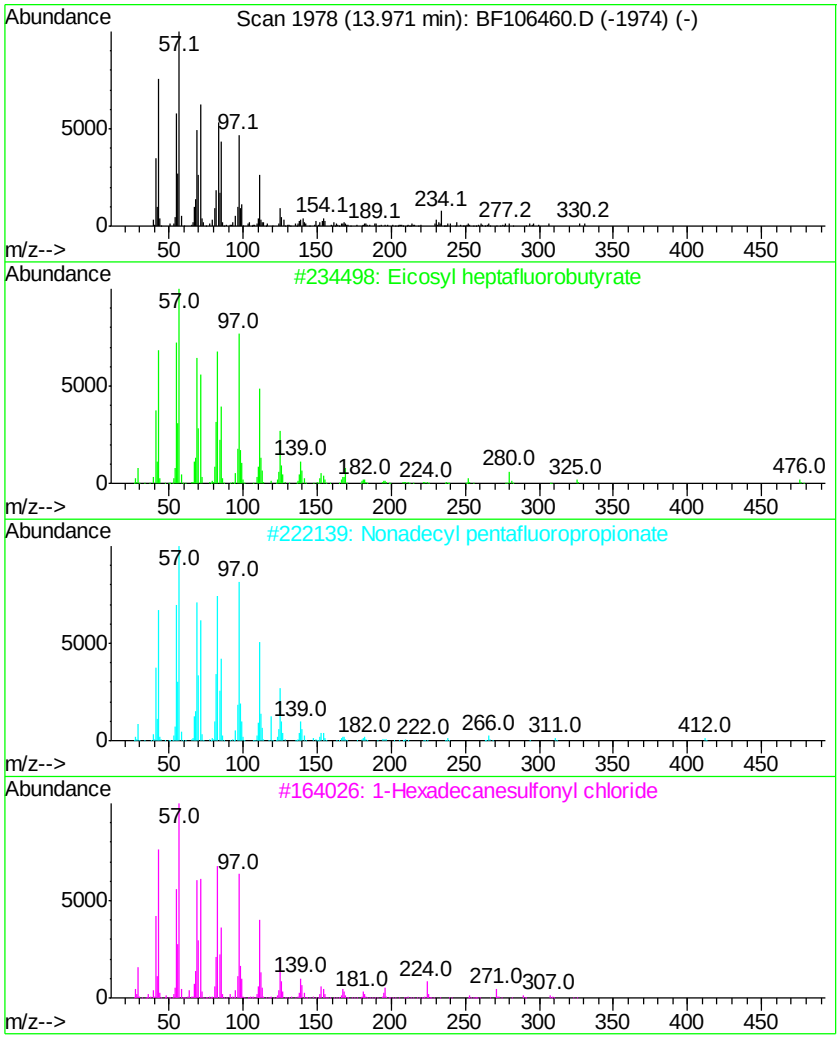
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

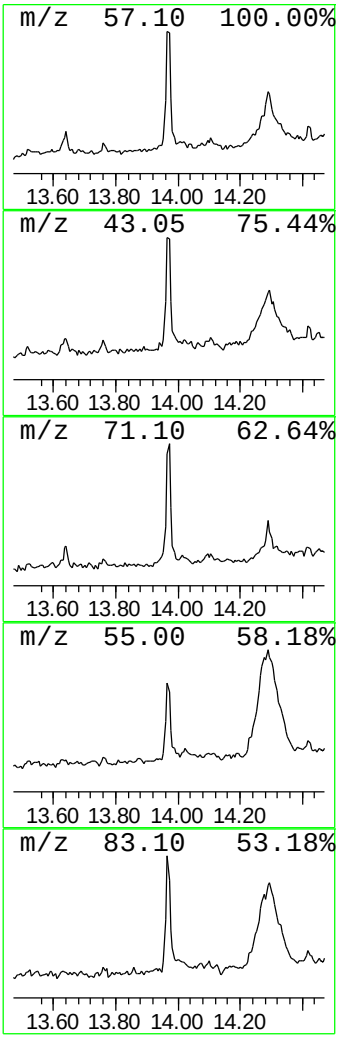
****

Peak Number 4 Eicosyl heptafluorobutyrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	6.12 ng	281180	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
4	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
5	E-7-Octadecene	252	C18H36	1000130-92-0	90





Library Search Compound Report

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Sample : J3471-04
Misc :
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Instrument : BNA_F
ClientSampleId : #2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

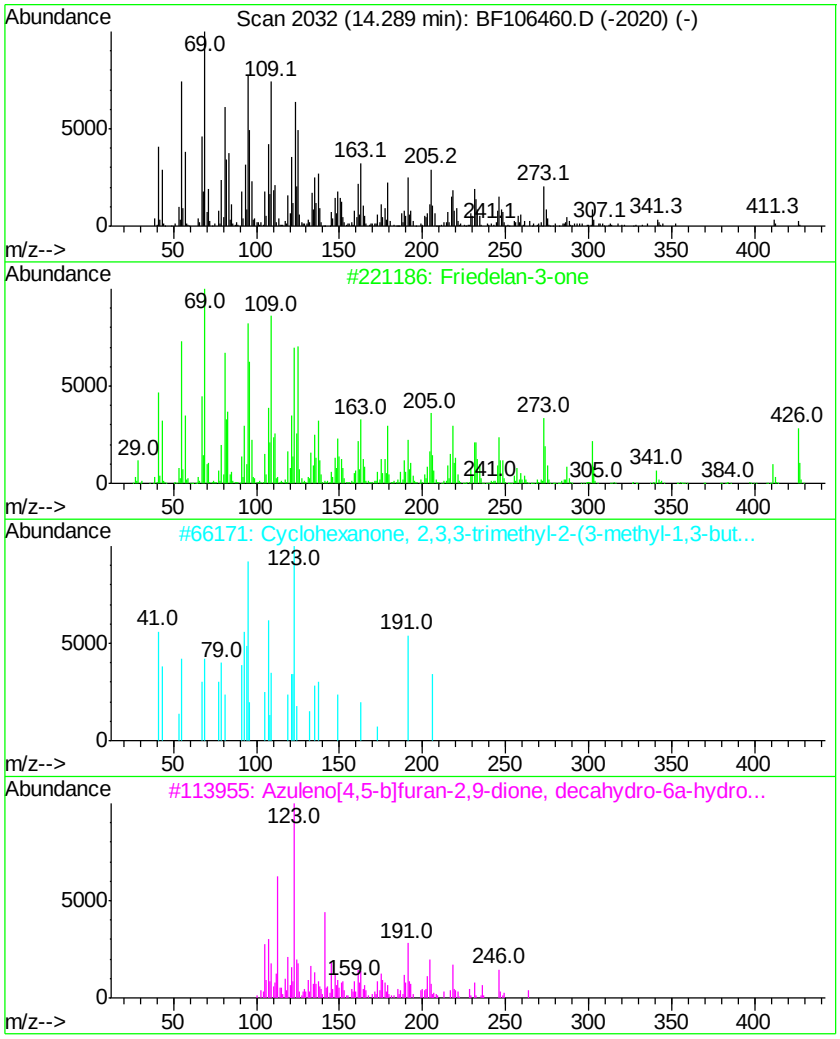
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

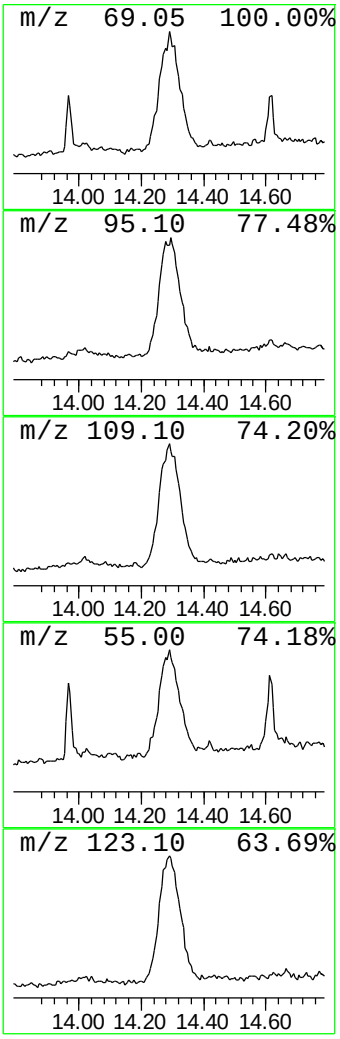
****

Peak Number 5 Friedelan-3-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	68.96 ng	3170430	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Friedelan-3-one	426	C30H50O	000559-74-0	99
2	Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	58
3	Azuleno[4,5-b]furan-2,9-dione, d...	264	C15H20O4	002571-81-5	56
4	D:A-Friedoursan-3-one	426	C30H50O	089950-00-5	45
5	3(4H)-Phenanthrenone, 4a,4b,5,6,...	246	C17H26O	057684-12-5	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
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Sample : J3471-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : #2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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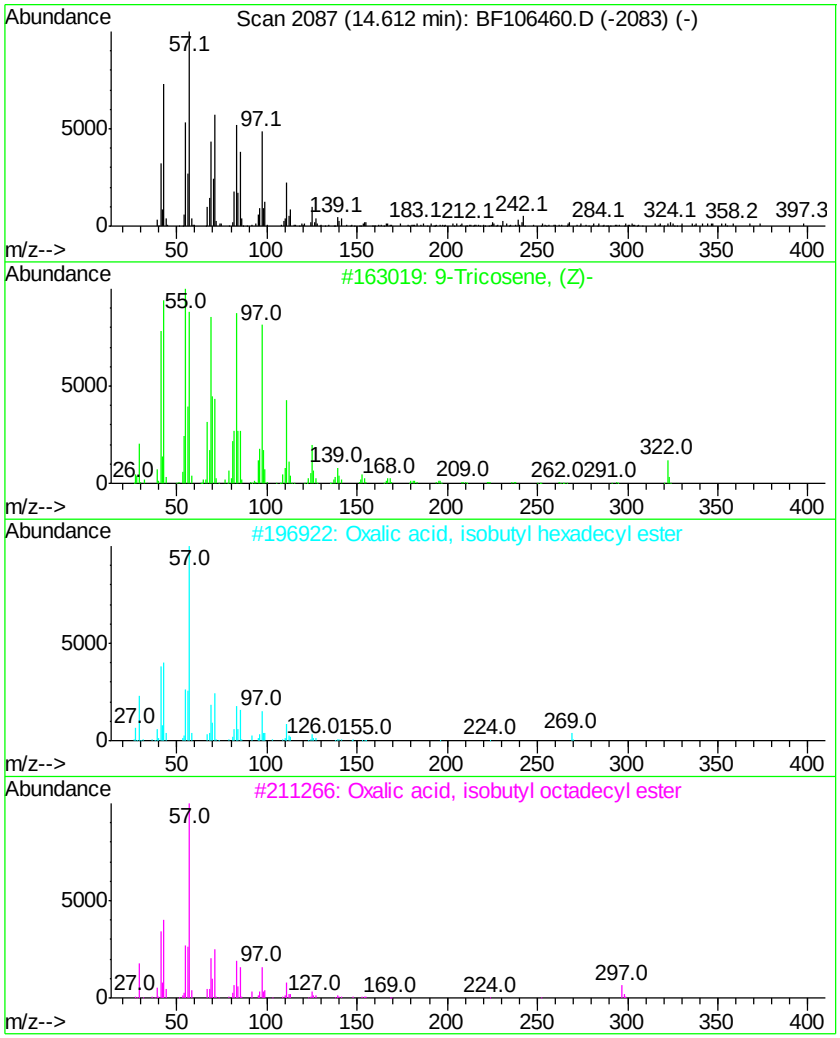
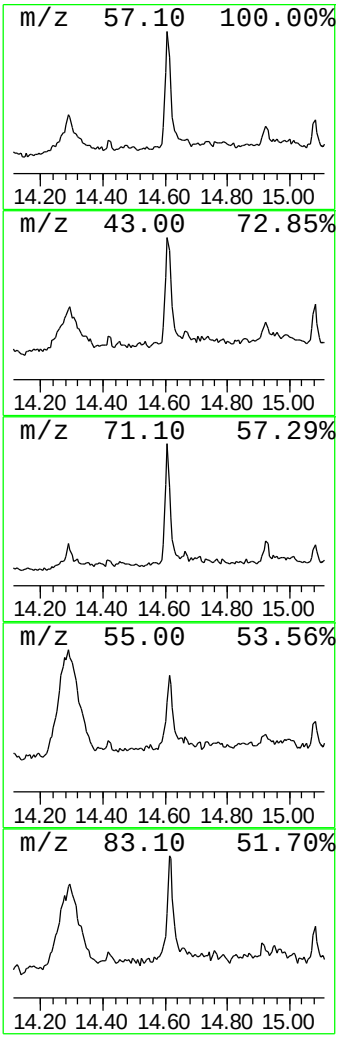
****

Peak Number 6 9-Tricosene, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	8.28 ng	380767	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-	322	C23H46	027519-02-4	93
2	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
3	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
4	Hexadecane, 1-(ethenyloxy)-	268	C18H36O	000822-28-6	81
5	Cyclotetracosane	336	C24H48	000297-03-0	78





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Misc :
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

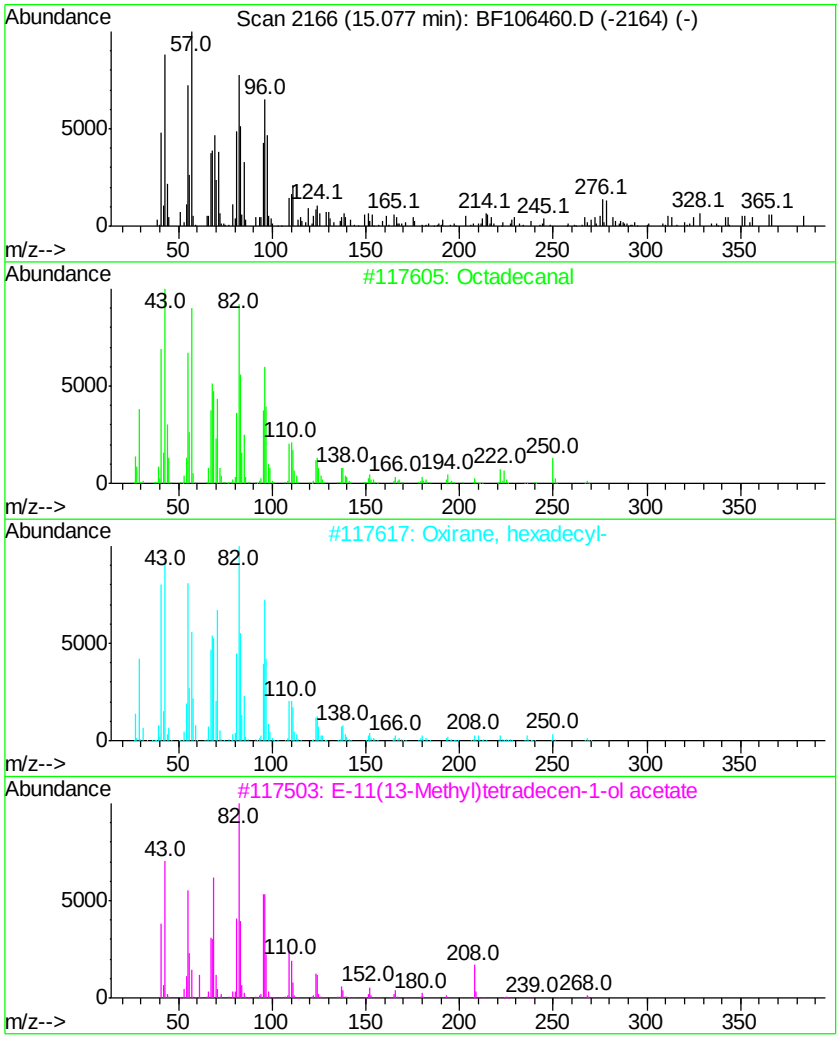
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

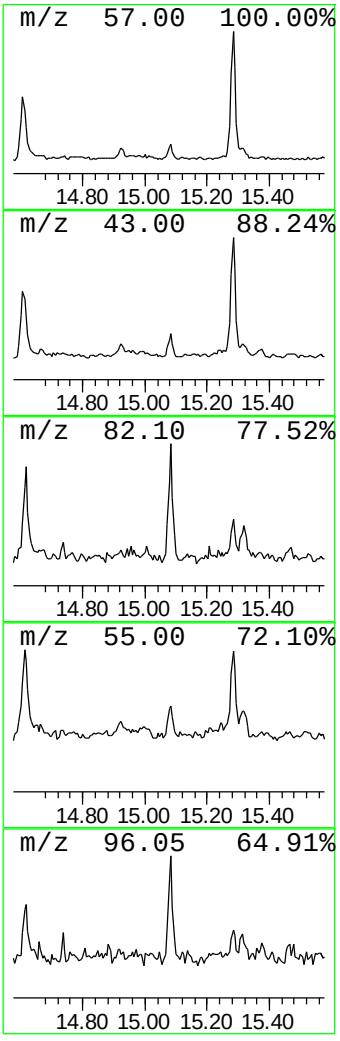
****

Peak Number 7 Octadecanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	4.58 ng	118392	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	93
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	93
3	E-11(13-Methyl)tetradecen-1-ol a...	268	C17H32O2	1000130-80-4	78
4	17-Octadecenal	266	C18H34O	056554-86-0	72
5	16-Octadecenal	266	C18H34O	056554-87-1	72





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : #2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

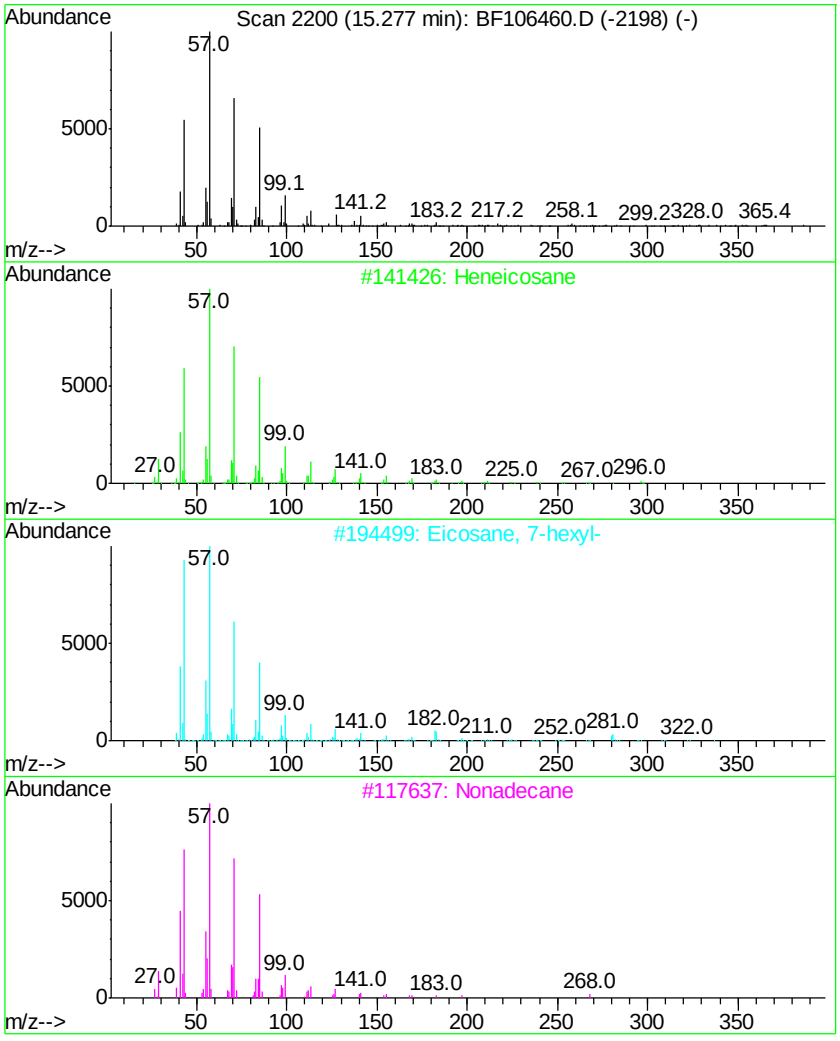
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

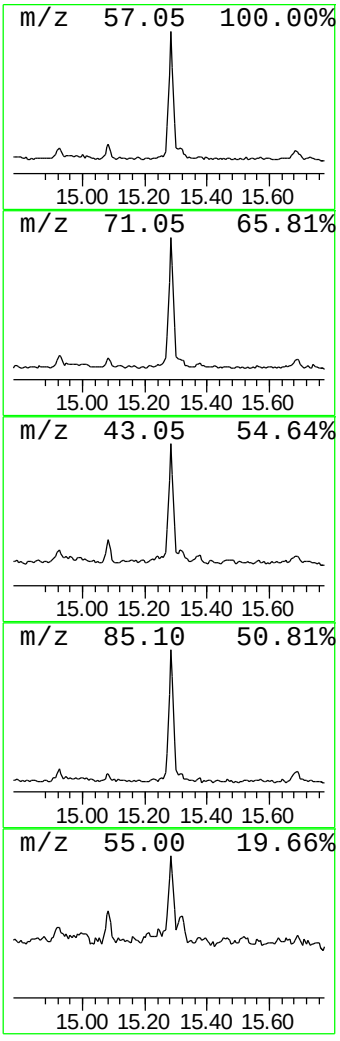
****

Peak Number 8 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	15.09 ng	390180	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
3	Nonadecane	268	C19H40	000629-92-5	87
4	Octacosane	394	C28H58	000630-02-4	81
5	Heptacosane	380	C27H56	000593-49-7	72





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Data File : BF106460.D
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Sample : J3471-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : #2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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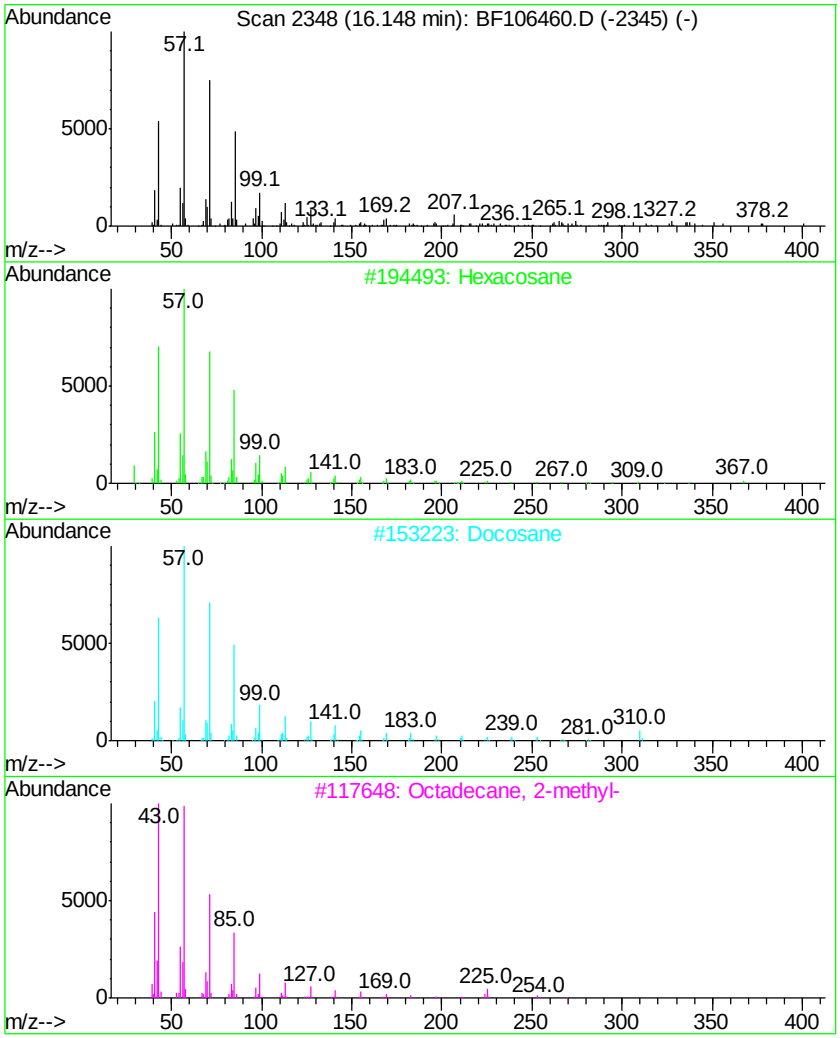
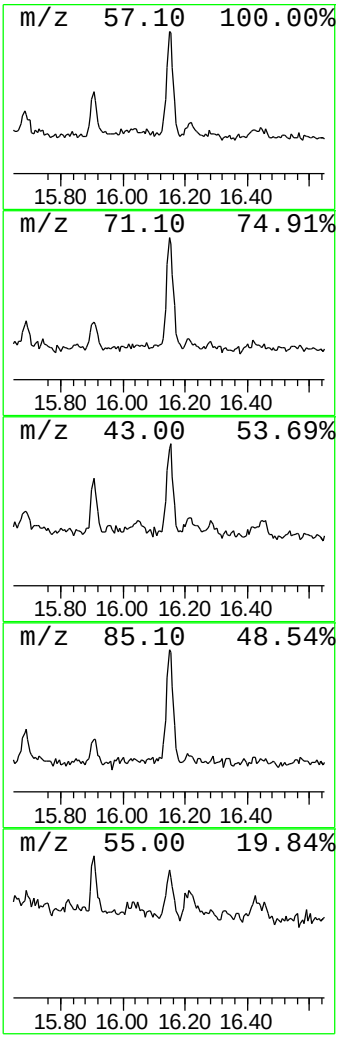
Peak Number 10 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	7.21 ng	186364	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Docosane	310	C22H46	000629-97-0	91
3	Octadecane, 2-methyl-	268	C19H40	001560-88-9	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061418\
Data File : BF106460.D
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Misc :
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.20	5.8	ng	217233	1	6.97	749089	20.0
unknown6.75	6.75	60.4	ng	2263540	1	6.97	749089	20.0
Eicosyl heptafluo...	13.97	6.1	ng	281180	5	14.15	919433	20.0
Friedelan-3-one	14.29	69.0	ng	3170430	5	14.15	919433	20.0
9-Tricosene, (Z)-	14.61	8.3	ng	380767	5	14.15	919433	20.0
Octadecanal	15.08	4.6	ng	118392	6	15.68	517227	20.0
Heneicosane	15.28	15.1	ng	390180	6	15.68	517227	20.0
Hexacosane	16.15	7.2	ng	186364	6	15.68	517227	20.0