LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109073.D
Acq On : 18 Sep 2018 3:33
Operator : JU/SJ
Sample : J4936-13
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26KV

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-BF091418.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	4.260	323	327	335	rBV	236232	298008	9.29%	1.075%
2	4.913	433	438	448	rVB	348990	437024	13.63%	1.577%
3	5.331	504	509	512	rBV	2784278	2792588	87.06%	10.075%
4	6.360	678	684	687	rBV	2928317	2964147	92.41%	10.694%
5	6.489	702	706	709	rBV	3235467	2909826	90.72%	10.498%
6	6.719	742	745	749	rBV	950862	764558	23.84%	2.758%
7	6.878	768	772	775	rBV	2845330	2424059	75.57%	8.746%
8	7.278	835	840	843	rBV	1878831	1871802	58.36%	6.753%
9	7.813	929	931	935	rVB	75330	64672	2.02%	0.233%
10	8.001	959	963	966	rBV	1121572	875601	27.30%	3.159%
11	9.078	1142	1146	1149	rBV	3799812	3207495	100.00%	11.572%
12	9.466	1209	1212	1216	rBV	209247	175368	5.47%	0.633%
13	9.748	1257	1260	1264	rBV2	1026810	875854	27.31%	3.160%
14	10.536	1390	1394	1406	rBV	1752493	1677842	52.31%	6.053%
15	11.224	1508	1511	1515	rBV	987980	869807	27.12%	3.138%
16	12.813	1776	1781	1784	rBV	3336100	3056246	95.28%	11.027%
17	13.718	1931	1935	1949	rBV2	126263	220050	6.86%	0.794%
18	13.854	1953	1958	1961	rBV	979285	928337	28.94%	3.349%
19	14.342	2038	2041	2047	rBV2	38286	41560	1.30%	0.150%
20	14.636	2088	2091	2094	rBV	55016	58566	1.83%	0.211%
21	14.707	2100	2103	2109	rVB	35213	36369	1.13%	0.131%
22	14.954	2142	2145	2149	rVB	64639	67149	2.09%	0.242%
23	15.254	2191	2196	2201	rBV	593731	666880	20.79%	2.406%
24	15.307	2201	2205	2211	rVB	73010	100819	3.14%	0.364%
25	15.712	2270	2274	2280	rVB	72801	95083	2.96%	0.343%
26	16.183	2349	2354	2363	rVB2	62231	115375	3.60%	0.416%
27	16.724	2441	2446	2454	rVB2	35033	69024	2.15%	0.249%
28	17.365	2551	2555	2563	rVB5	24655	53101	1.66%	0.192%

Sum of corrected areas: 27717210

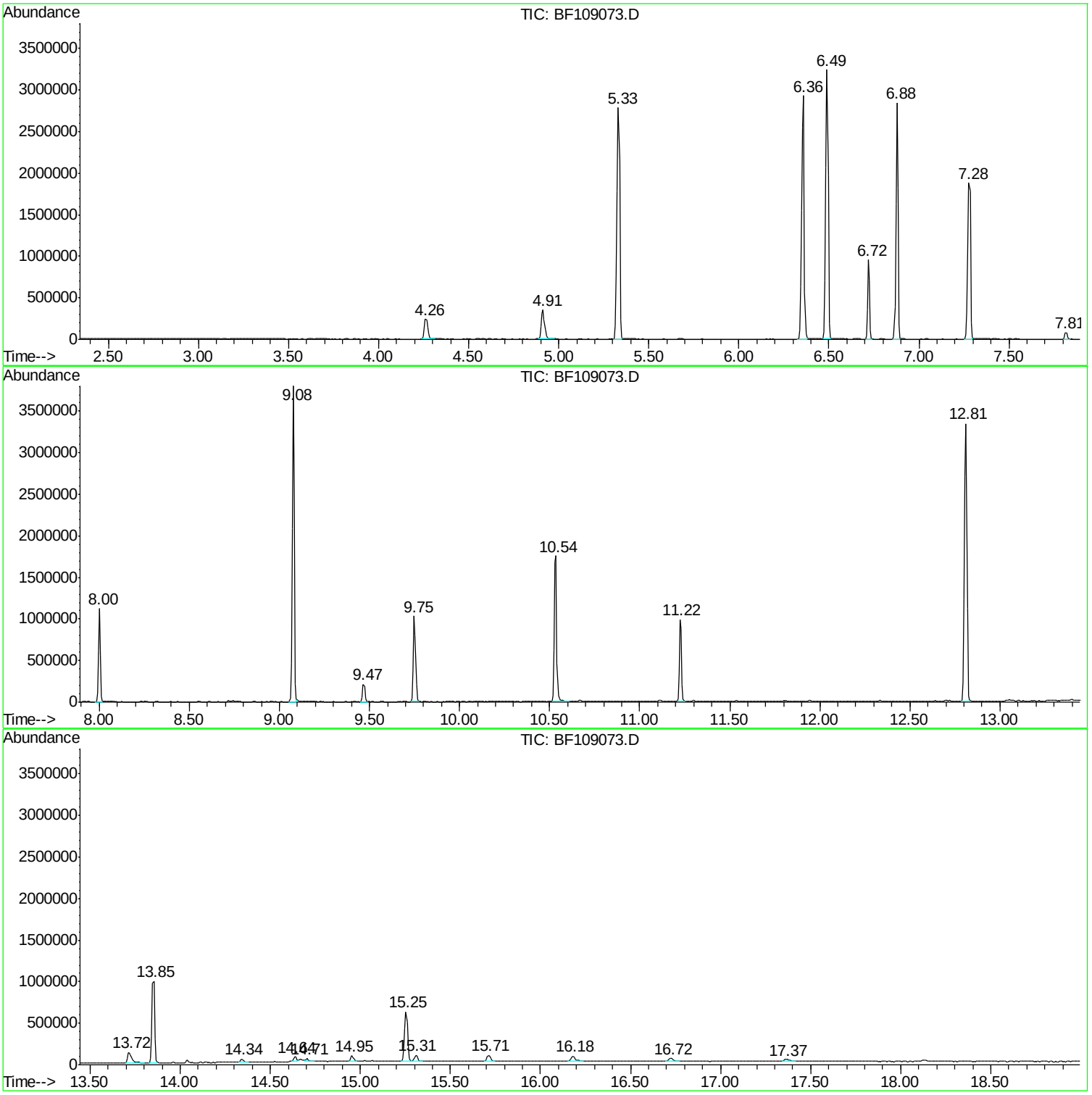
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109073.D
Acq On : 18 Sep 2018 3:33
Operator : JU/SJ
Sample : J4936-13
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26KV

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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

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Data File : BF109073.D
Acq On : 18 Sep 2018 3:33
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

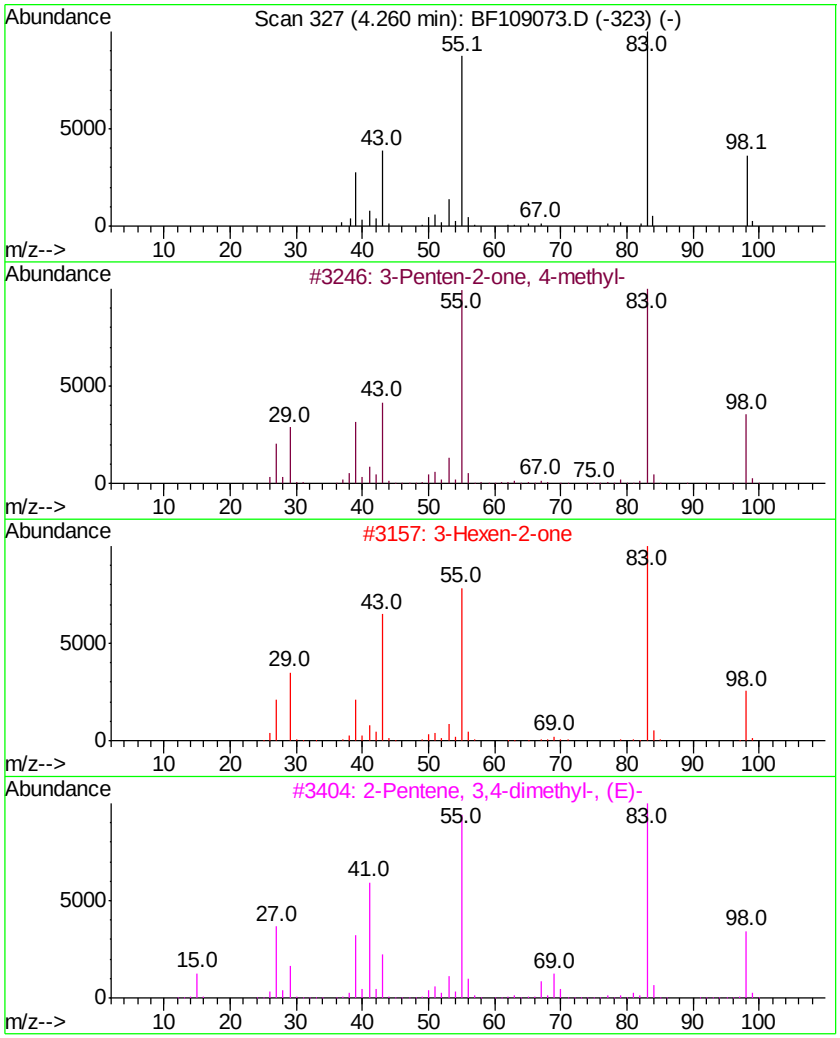
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

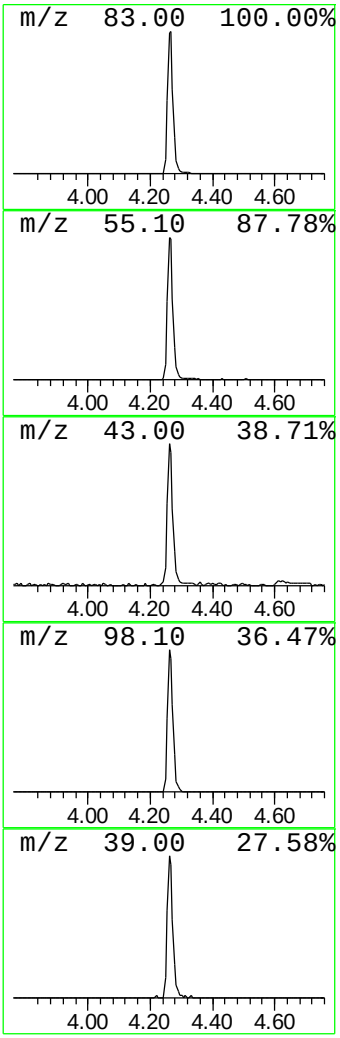
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.26	7.80 ng	298008	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78





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Operator : JU/SJ
Sample : J4936-13
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26KV

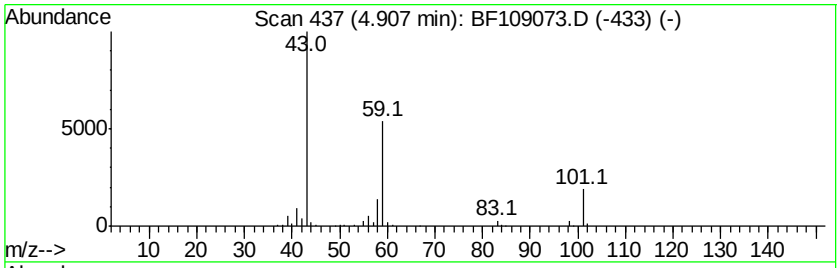
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

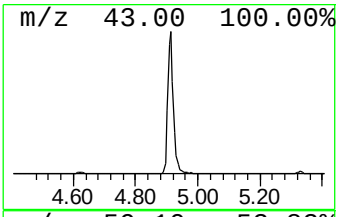
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

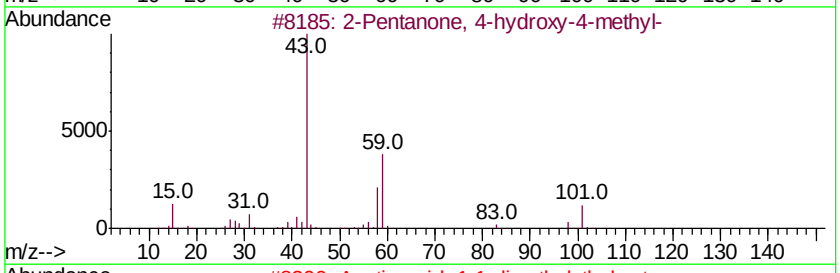
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

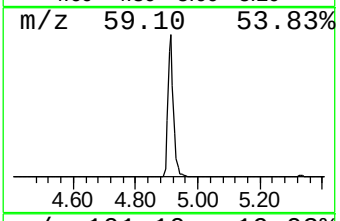
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	11.43 ng	437024	1,4-Dichlorobenzene-d4	6.72

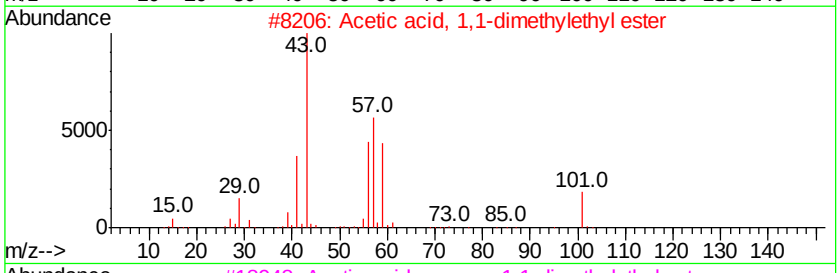
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9

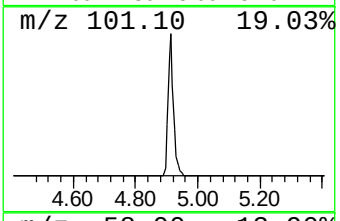


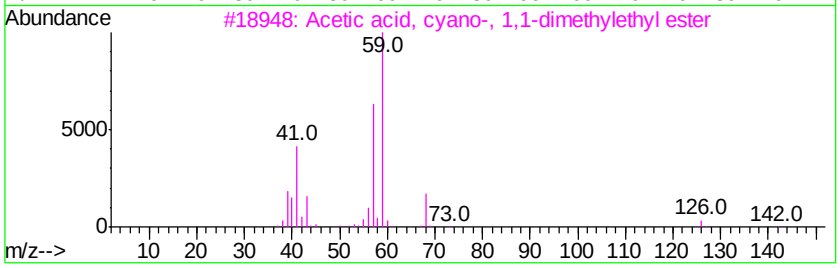


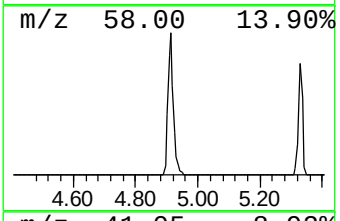


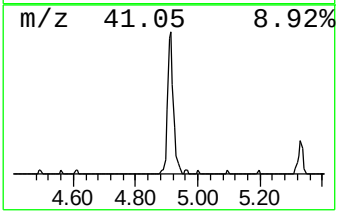












Library Search Compound Report

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Operator : JU/SJ
Sample : J4936-13
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26KV

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

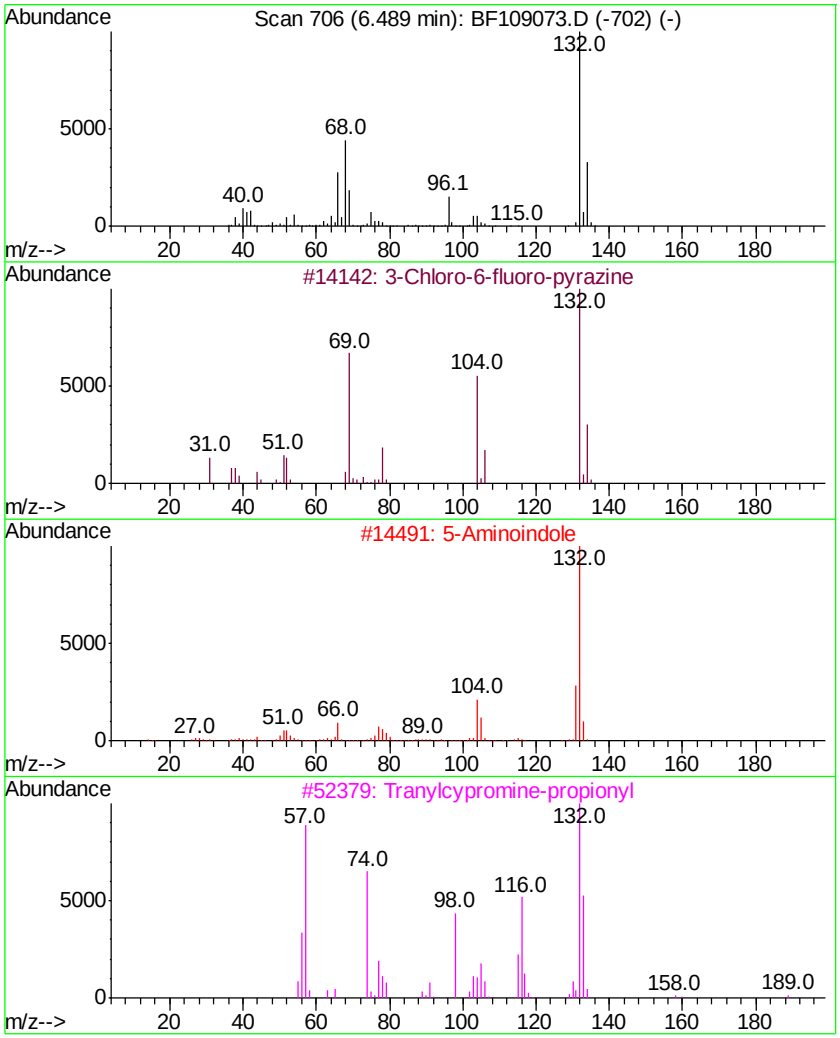
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

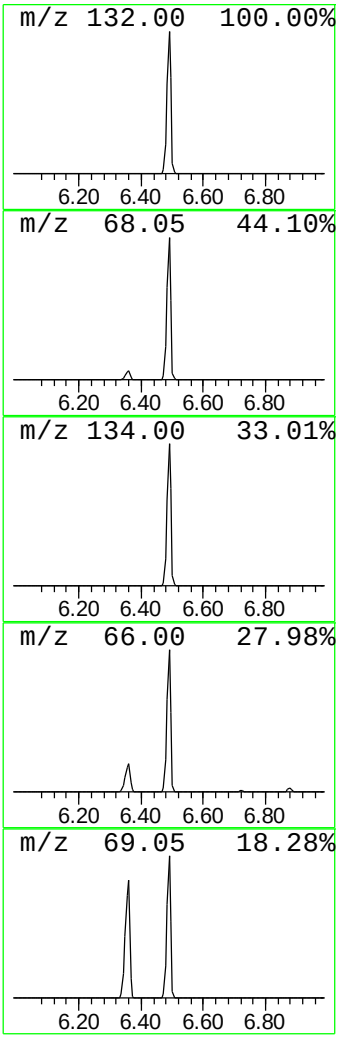
****

Peak Number 3 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	76.12 ng	2909830	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





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Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26KV

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
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TIC Library : C:\DATABASE\NIST11.L
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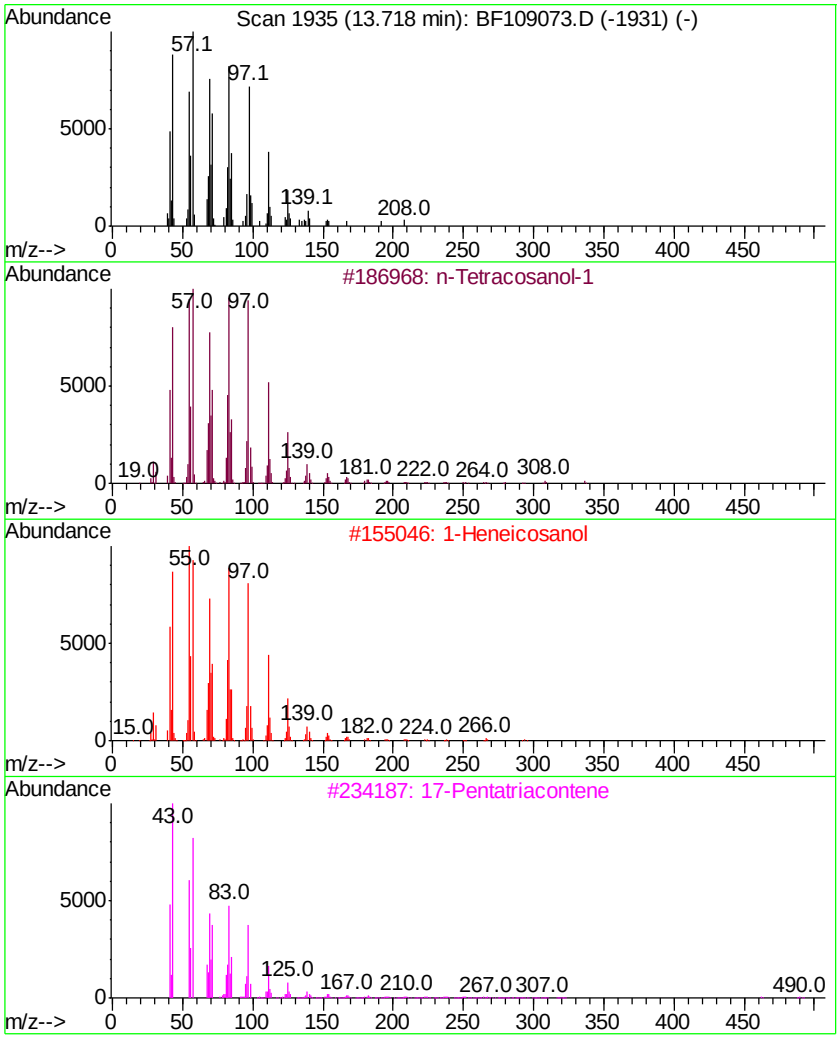
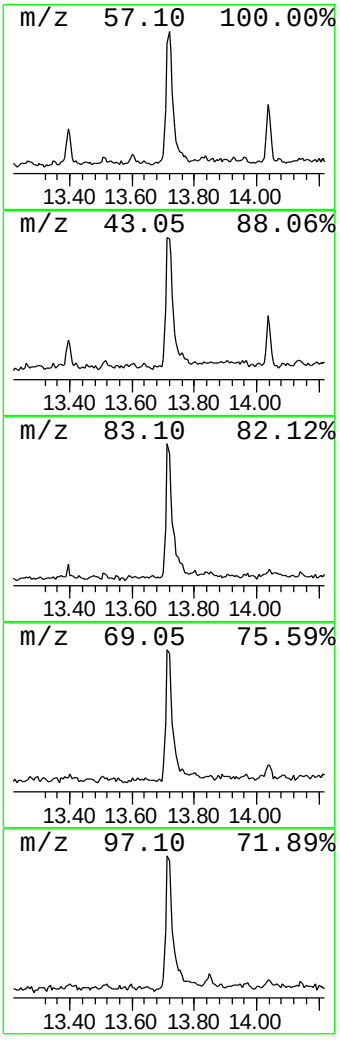
****

Peak Number 5 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	4.74 ng	220050	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	17-Pentatriacontene	491	C35H70	006971-40-0	91
4	Behenic alcohol	326	C22H46O	000661-19-8	90
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	87





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ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26KV

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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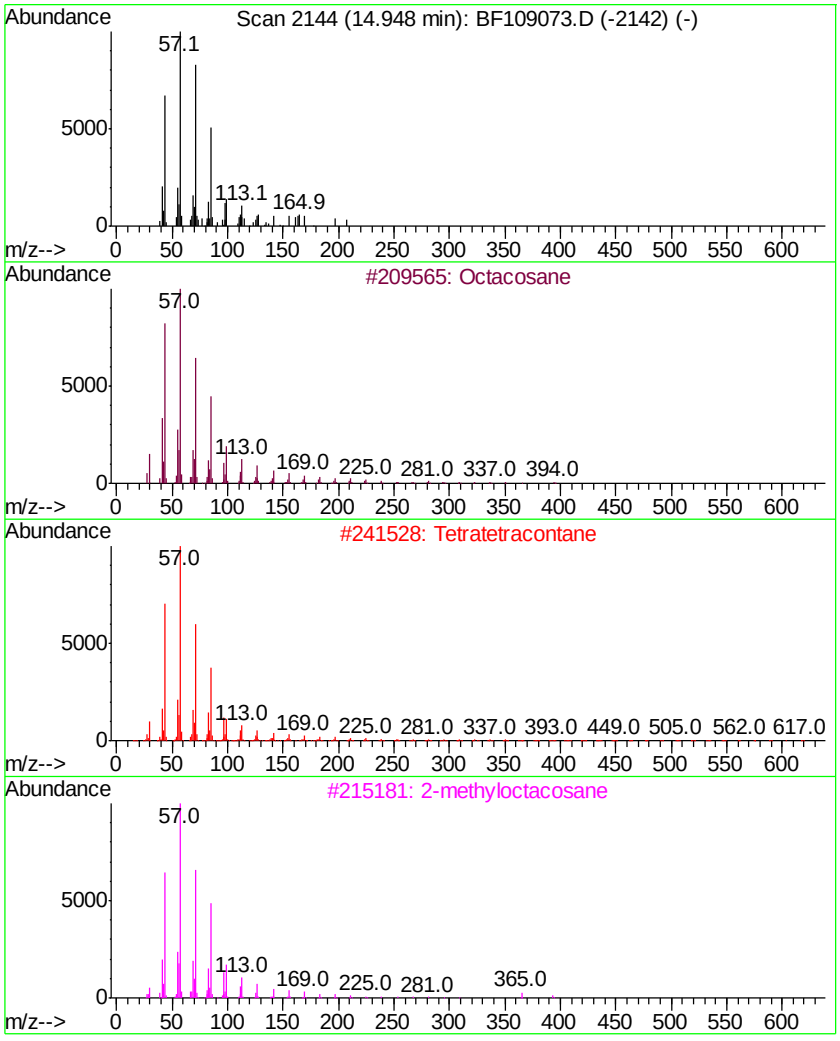
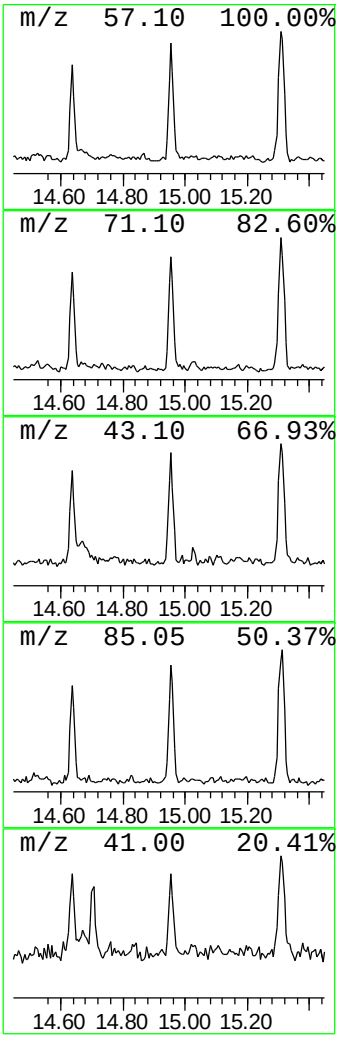
****

Peak Number 6 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	2.01 ng	67149	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Hentriacontane	437	C31H64	000630-04-6	91
5	Triacontane	422	C30H62	000638-68-6	91





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Instrument : BNA_F
ClientSampleId : 26KV

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

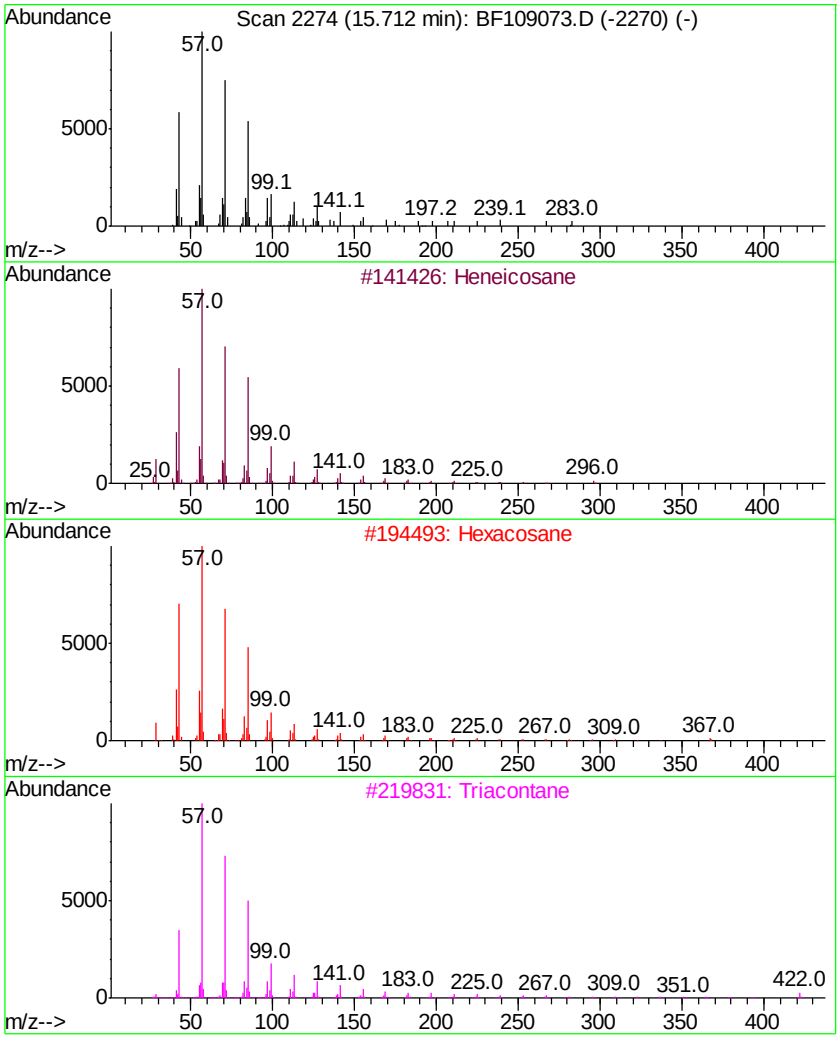
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

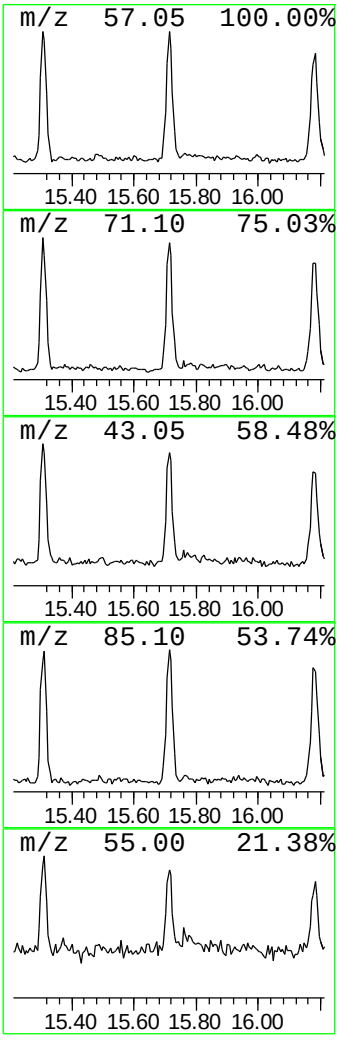
****

Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	2.85 ng	95083	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Docosane	310	C22H46	000629-97-0	91





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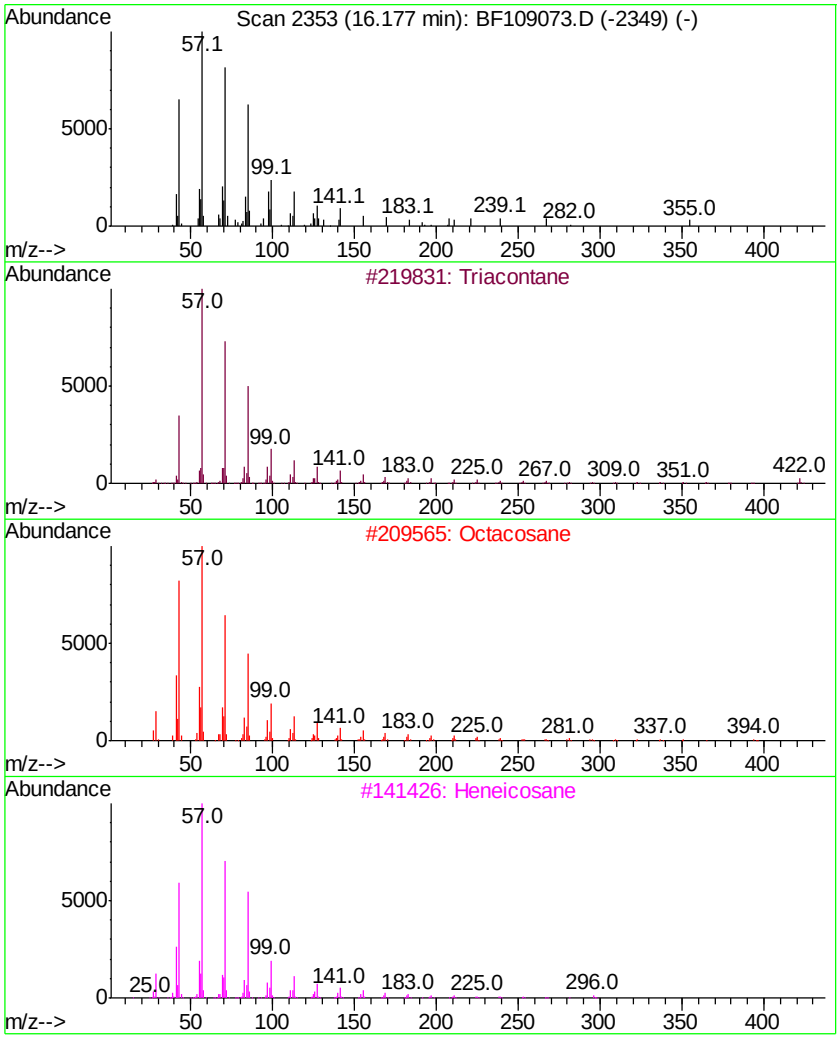
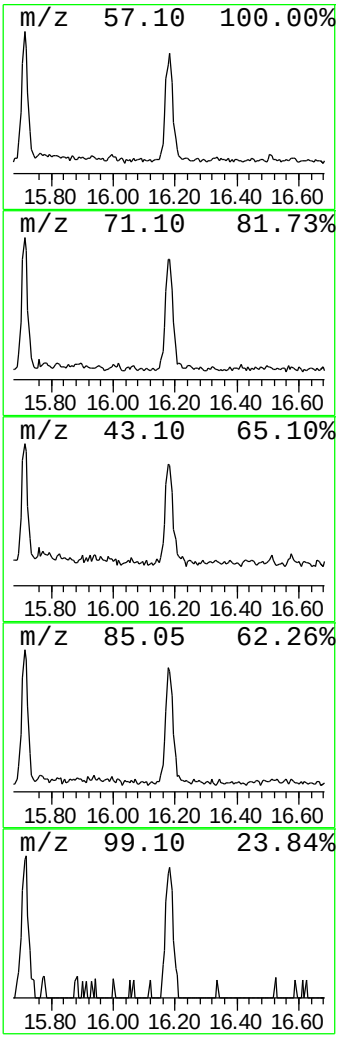
****

Peak Number 9 Triacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	3.46 ng	115375	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Octacosane	394	C28H58	000630-02-4	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	2-methyloctacosane	408	C29H60	1000376-72-8	87
5	Pentacosane	352	C25H52	000629-99-2	87





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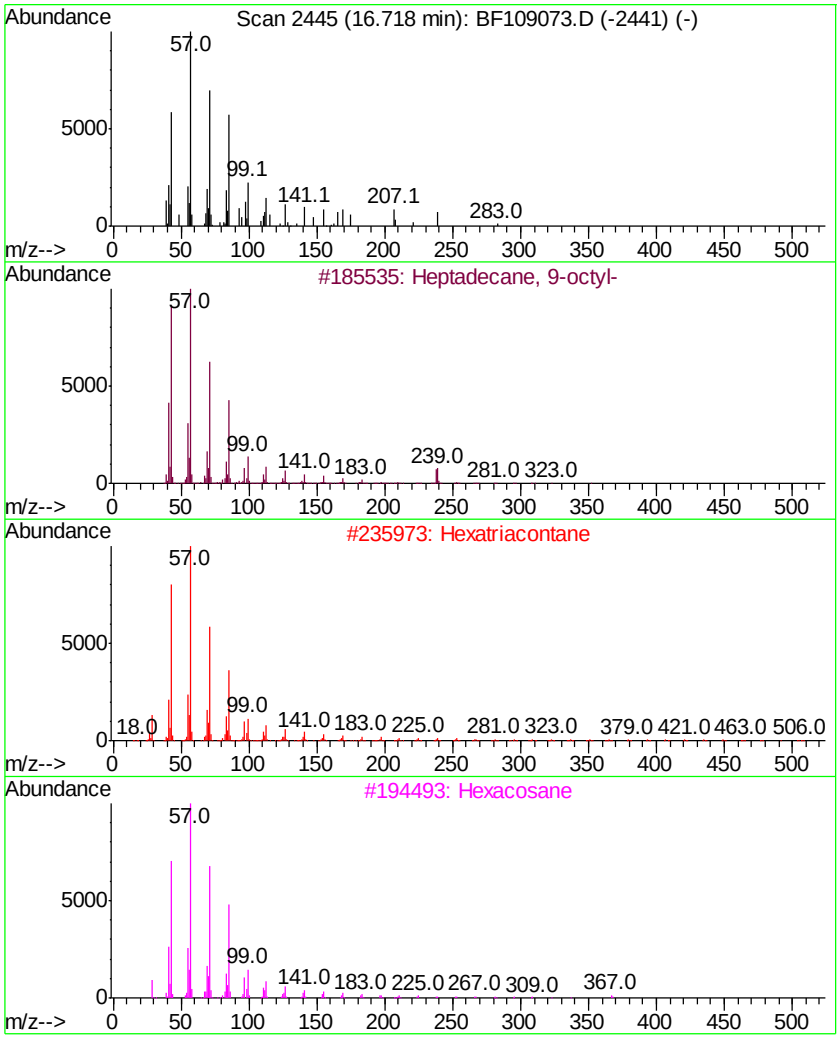
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

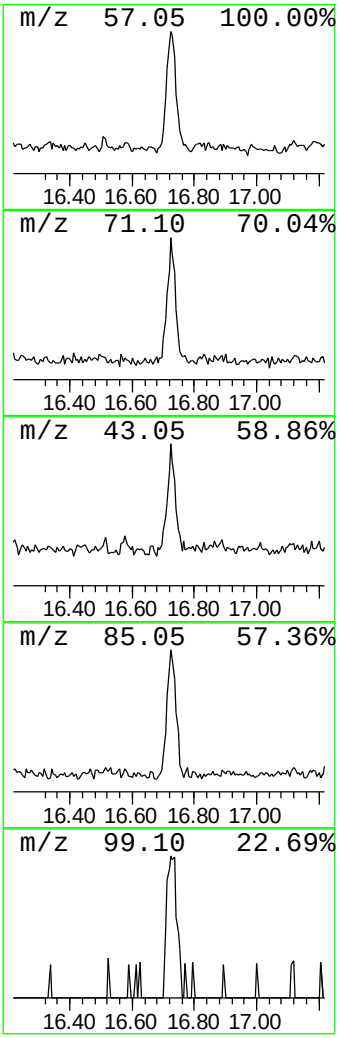
****

Peak Number 10 Heptadecane, 9-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	2.07 ng	69024	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Hexatriacontane	507	C36H74	000630-06-8	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Triacontane	422	C30H62	000638-68-6	90
5	Heptacosane	380	C27H56	000593-49-7	90





Tentatively Identified Compound (LSC) summary

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Sample : J4936-13
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26KV

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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
3-Penten-2-one, 4...	4.26	7.8	ng	298008	1	6.72	764558	20.0
2-Pentanone, 4-hy...	4.91	11.4	ng	437024	1	6.72	764558	20.0
unknown6.49	6.49	76.1	ng	2909830	1	6.72	764558	20.0
n-Tetracosanol-1	13.72	4.7	ng	220050	5	13.85	928337	20.0
Octacosane	14.95	2.0	ng	67149	6	15.25	666880	20.0
Heneicosane	15.71	2.9	ng	95083	6	15.25	666880	20.0
Triacontane	16.18	3.5	ng	115375	6	15.25	666880	20.0
Heptadecane, 9-oc...	16.72	2.1	ng	69024	6	15.25	666880	20.0