LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080219\
Data File : BF115938.D
Acq On : 2 Aug 2019 11:20
Operator : HP/JU
Sample : PB121939BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB121939BL

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-BF073019.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	2.210	12	21	29	rVB	62979	94920	2.03%	0.274%
2	5.081	505	509	521	rBV	211059	302270	6.48%	0.874%
3	5.487	573	578	596	rBV	2566757	2699304	57.83%	7.802%
4	6.487	743	748	763	rBV	2615465	2682933	57.48%	7.755%
5	6.622	767	771	775	rBV	2938623	2875734	61.61%	8.312%
6	6.851	806	810	819	rBV	1136654	943639	20.22%	2.728%
7	7.010	832	837	840	rBV	3406756	3172169	67.96%	9.169%
8	7.416	900	906	909	rBV	2322643	2530998	54.22%	7.316%
9	8.133	1023	1028	1046	rBV	1197910	1197526	25.65%	3.461%
10	9.216	1205	1212	1215	rBV	4280681	4555368	97.59%	13.167%
11	9.892	1322	1327	1348	rBV	1484508	1423309	30.49%	4.114%
12	10.680	1457	1461	1486	rBV	1848272	2099888	44.99%	6.070%
13	11.380	1576	1580	1601	rVB	1536464	1454532	31.16%	4.204%
14	12.968	1845	1850	1853	rBV	4536521	4667930	100.00%	13.492%
15	14.021	2025	2029	2042	rVB	1262578	1284512	27.52%	3.713%
16	14.480	2102	2107	2112	rBV2	86033	88133	1.89%	0.255%
17	14.786	2154	2159	2166	rBV	183738	196160	4.20%	0.567%
18	15.127	2211	2217	2225	rBV	239265	298258	6.39%	0.862%
19	15.498	2274	2280	2294	rBV2	864448	1451743	31.10%	4.196%
20	15.939	2349	2355	2363	rVB	190280	304077	6.51%	0.879%
21	16.439	2434	2440	2454	rVB	108753	198167	4.25%	0.573%
22	17.033	2534	2541	2551	rBV3	33723	75573	1.62%	0.218%

Sum of corrected areas: 34597143

LSC Report - Integrated Chromatogram

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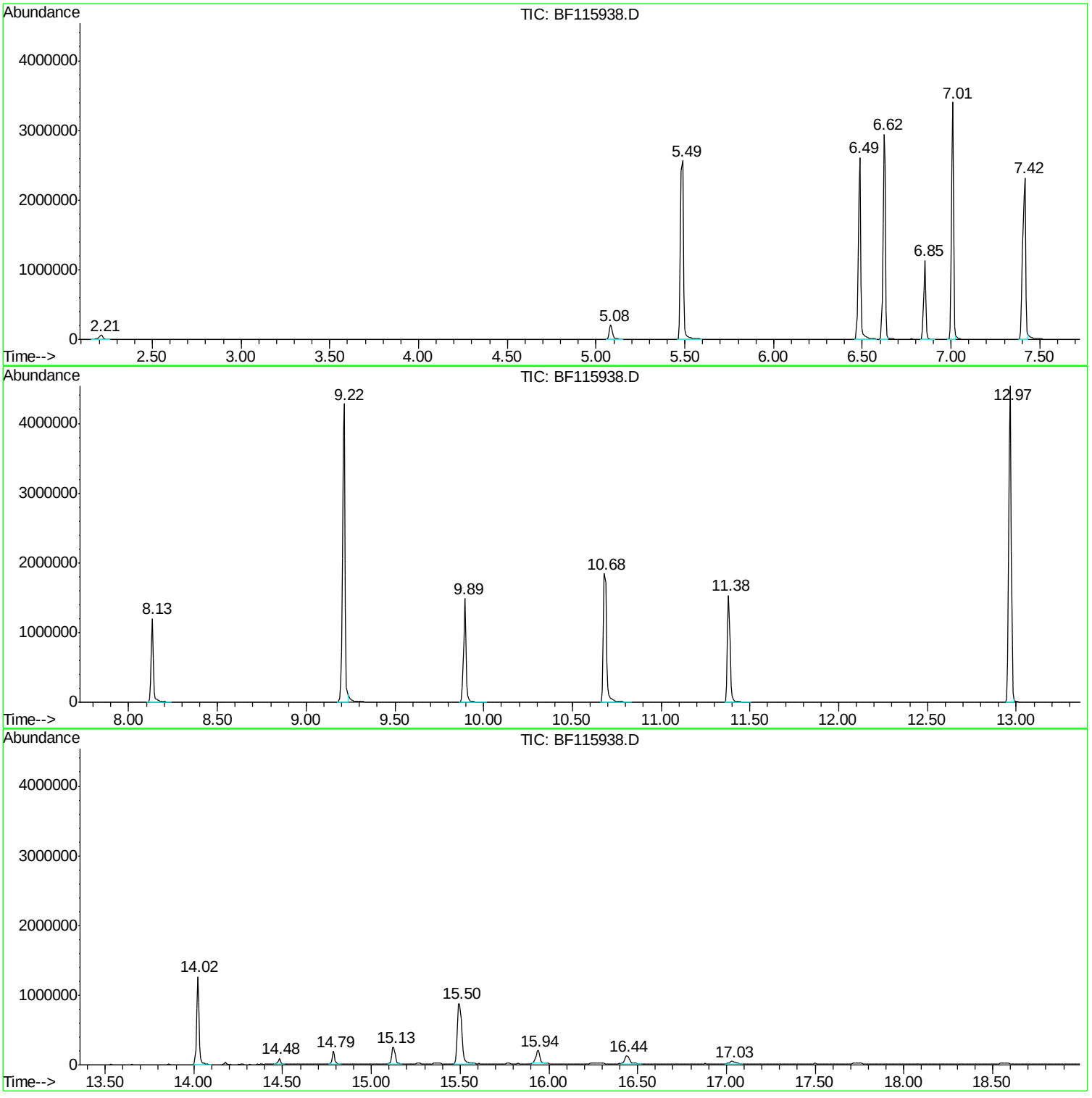
Sample : PB121939BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB121939BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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\BF080219\
Data File : BF115938.D
Acq On : 2 Aug 2019 11:20
Operator : HP/JU
Sample : PB121939BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB121939BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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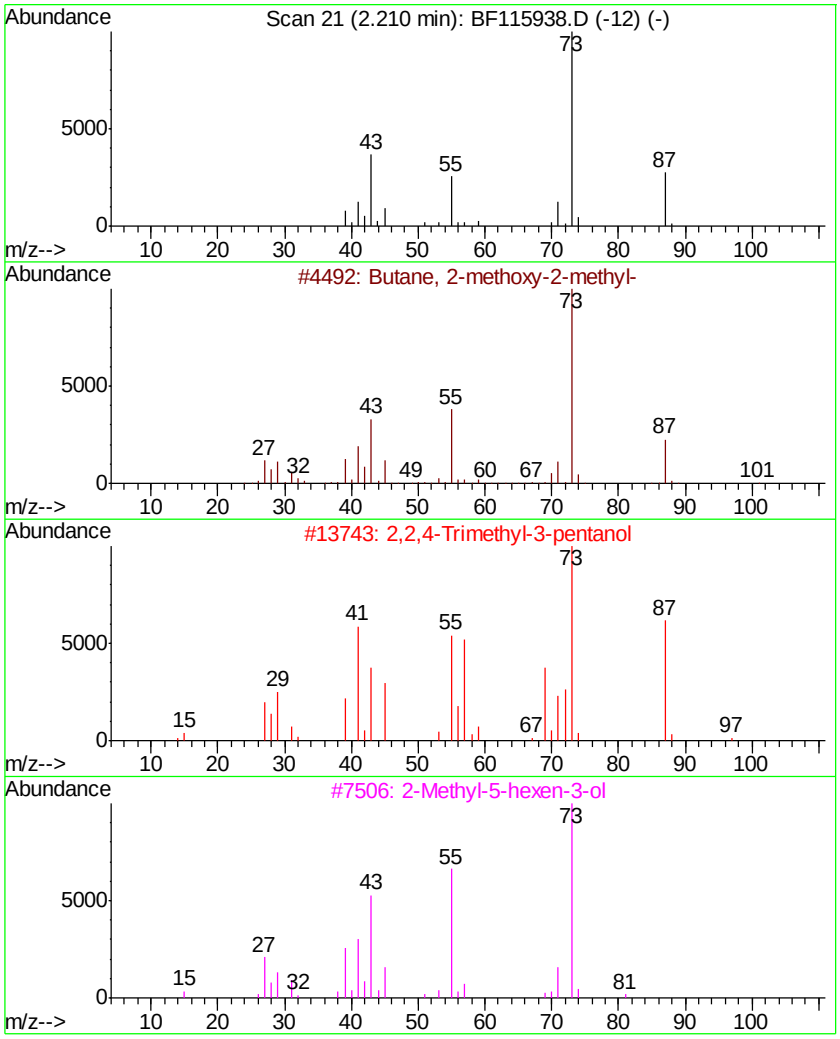
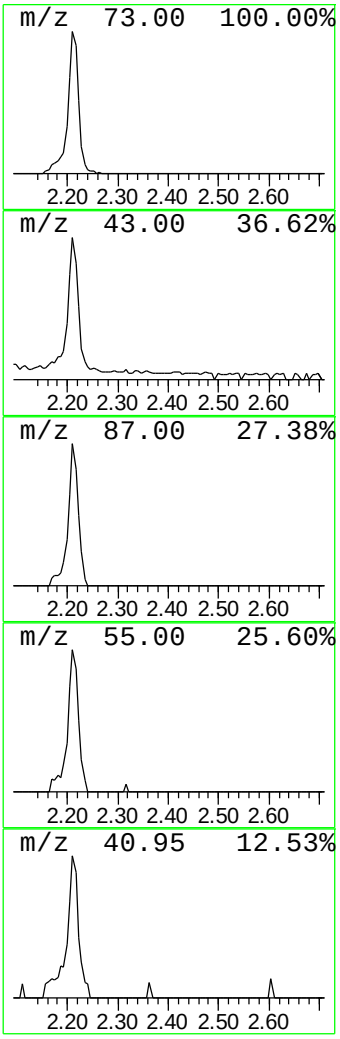
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.21	2.01 ng	94920	1,4-Dichlorobenzene-d4	6.85

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	40
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	17
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12





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Acq On : 2 Aug 2019 11:20
Operator : HP/JU
Sample : PB121939BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB121939BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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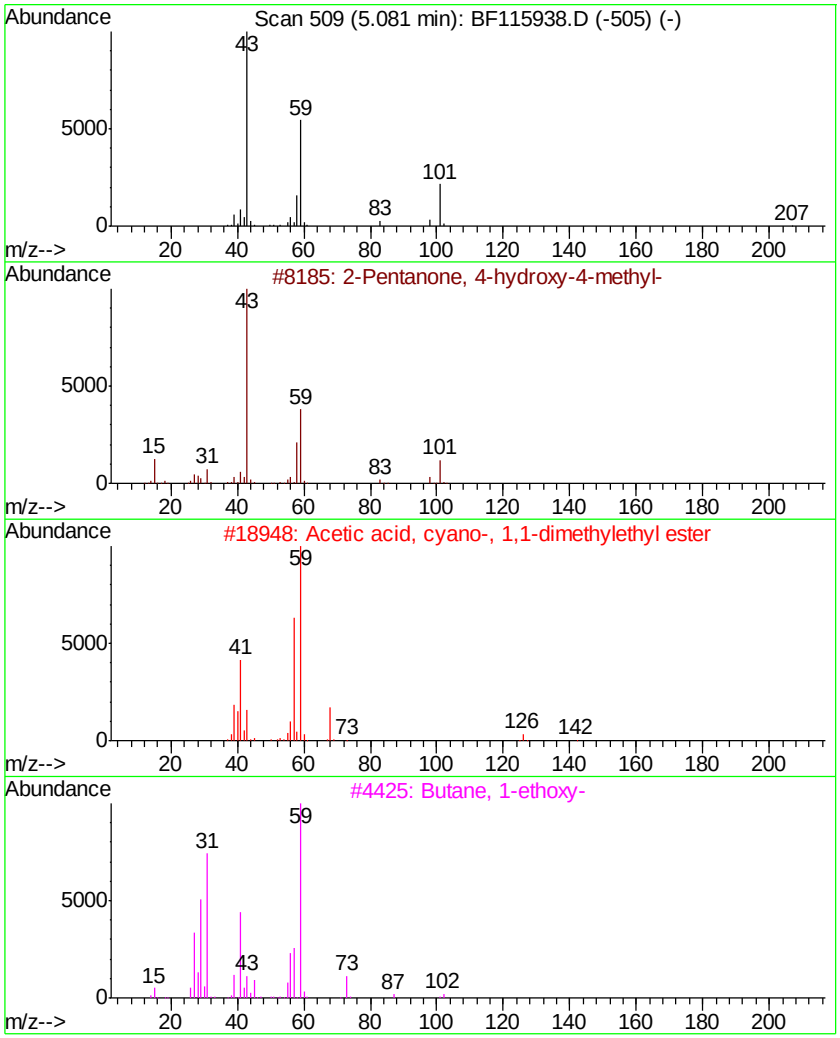
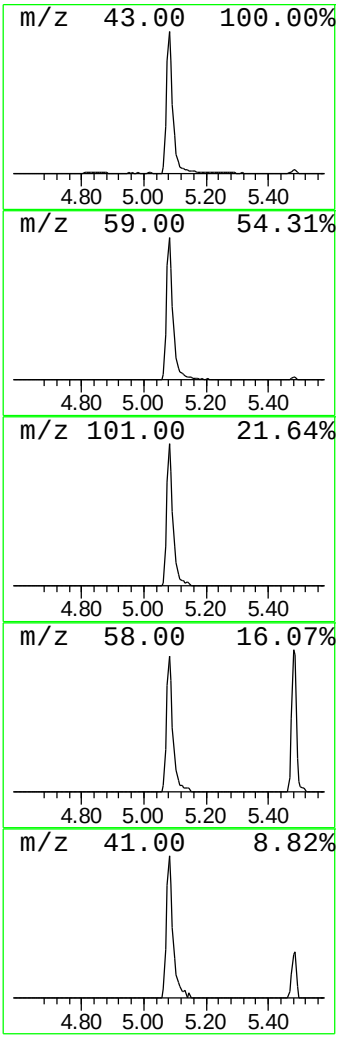
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	6.41 ng	302270	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane	58	C4H10	000106-97-8	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080219\
Data File : BF115938.D
Acq On : 2 Aug 2019 11:20
Operator : HP/JU
Sample : PB121939BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB121939BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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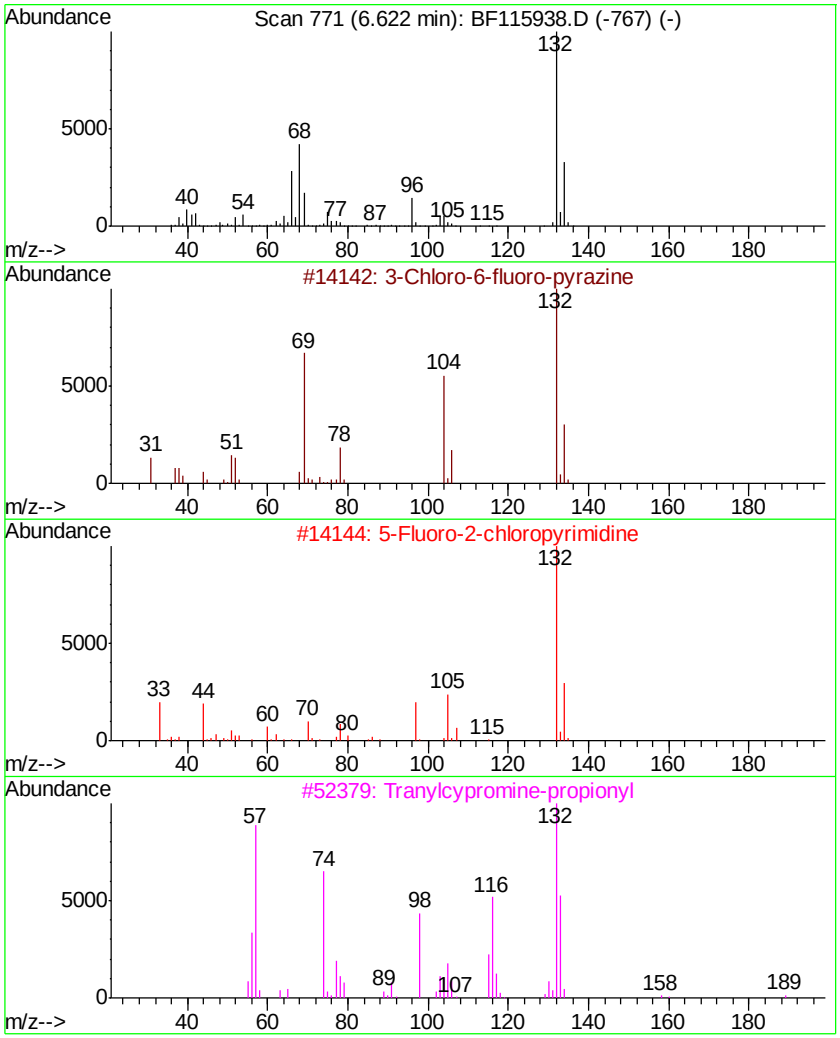
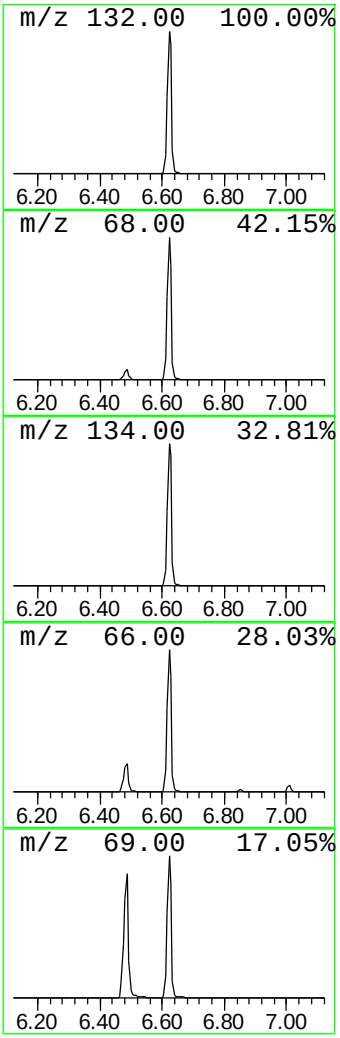
Peak Number 3 unknown6.62 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	60.95 ng	2875730	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080219\
Data File : BF115938.D
Acq On : 2 Aug 2019 11:20
Operator : HP/JU
Sample : PB121939BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB121939BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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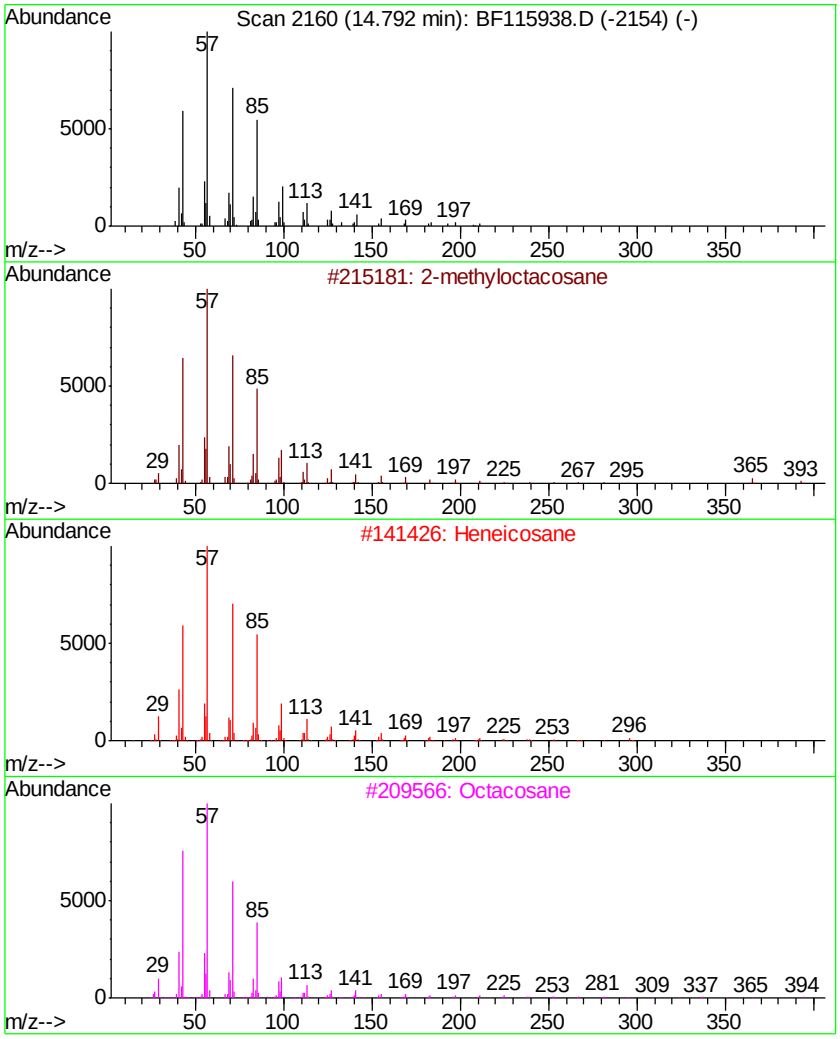
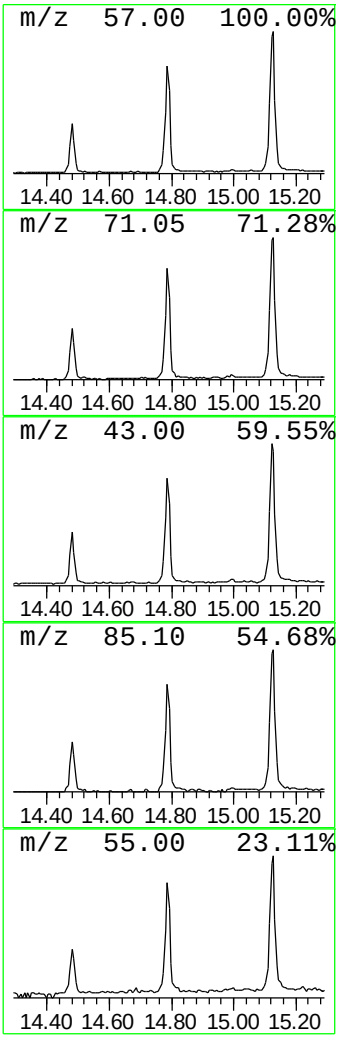
Peak Number 5 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	2.70 ng	196160	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	86





Library Search Compound Report

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Operator : HP/JU
Sample : PB121939BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB121939BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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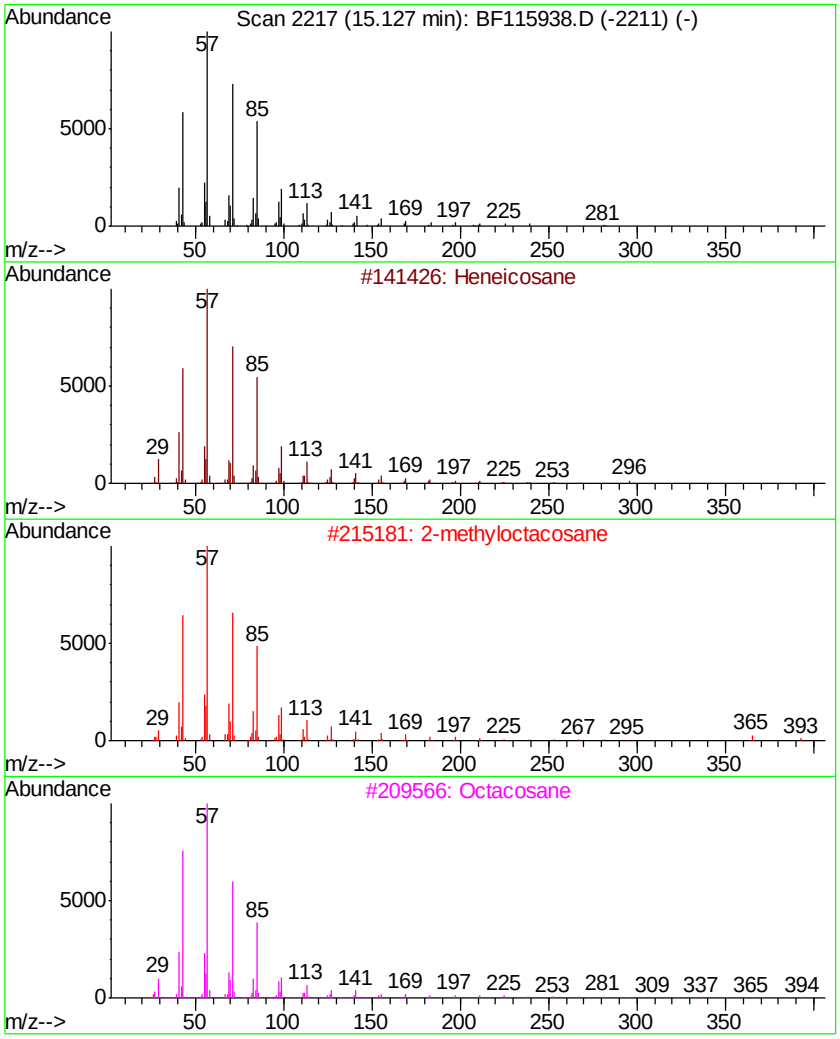
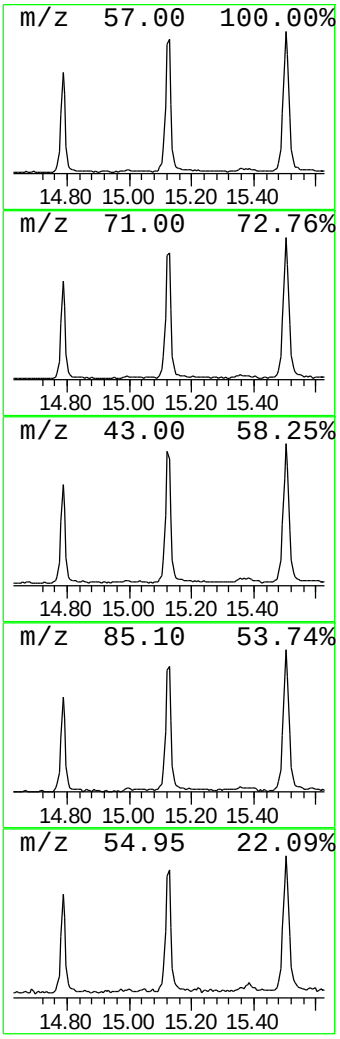
Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	4.11 ng	298258	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Hentriacontane	437	C31H64	000630-04-6	91





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Sample : PB121939BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB121939BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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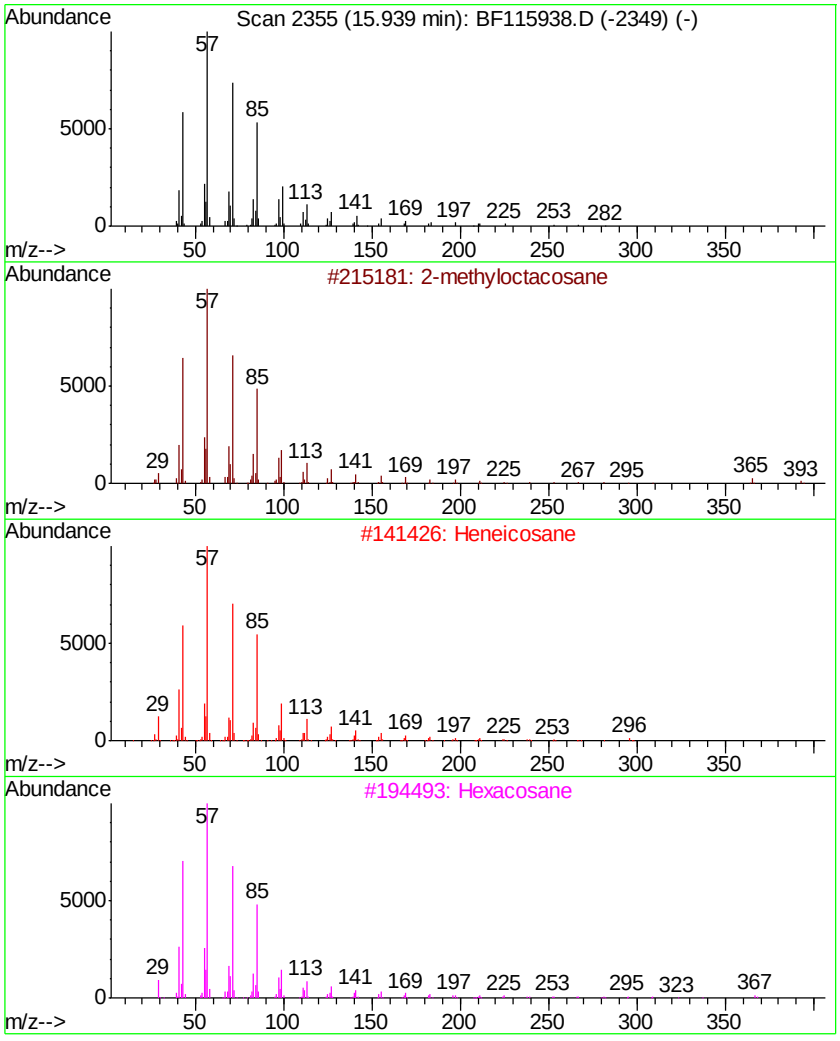
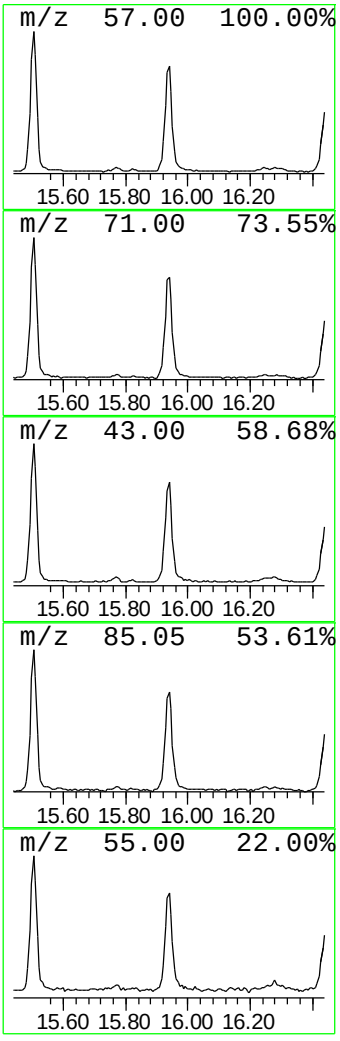
Peak Number 7 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	4.19 ng	304077	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexacosane	366	C26H54	000630-01-3	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87





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Instrument : BNA_F
ClientSampleId : PB121939BL

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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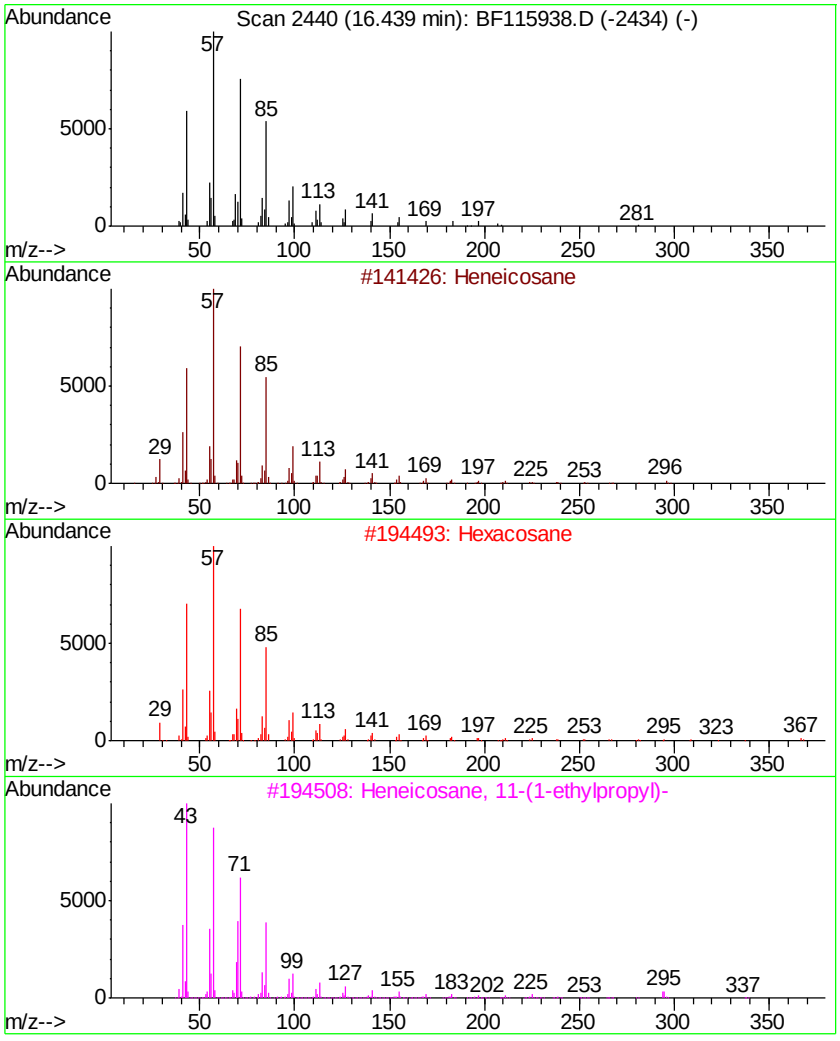
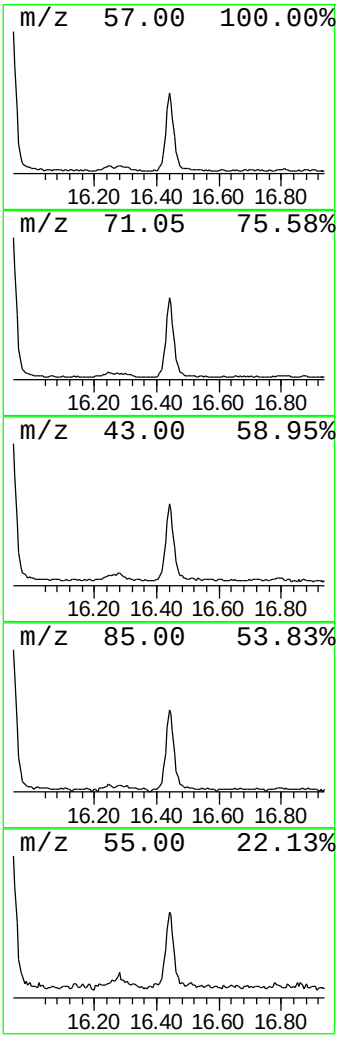
Peak Number 8 Heneicosane, 11-(1-ethylpro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.44	2.73 ng	198167	Perylene-d12	15.49

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	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Triacontane	422	C30H62	000638-68-6	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080219\
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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
Butane, 2-methoxy...	2.21	2.0	ng	94920	1	6.85	943639	20.0
2-Pentanone, 4-hy...	5.08	6.4	ng	302270	1	6.85	943639	20.0
unknown6.62	6.62	61.0	ng	2875730	1	6.85	943639	20.0
2-methyloctacosane	14.79	2.7	ng	196160	6	15.49	1451740	20.0
Heneicosane	15.13	4.1	ng	298258	6	15.49	1451740	20.0
Hexacosane	15.94	4.2	ng	304077	6	15.49	1451740	20.0
Heneicosane, 11-(...	16.44	2.7	ng	198167	6	15.49	1451740	20.0