LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052219\
Data File : BF114491.D
Acq On : 22 May 2019 19:01
Operator : JU/SJ
Sample : K2962-10
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-4

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-BF051019.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	5.457	570	573	600	rBV	2456070	2976612	92.69%	8.749%
2	6.475	742	746	764	rBV	2926266	3184759	99.17%	9.361%
3	6.604	764	768	780	rVB	3469401	3029753	94.35%	8.905%
4	6.828	803	806	817	rBV	1184010	970775	30.23%	2.853%
5	6.987	829	833	846	rBV	2457124	2303522	71.73%	6.771%
6	7.392	898	902	920	rBV	1848183	1942950	60.50%	5.711%
7	8.110	1020	1024	1044	rBV	1206171	1268157	39.49%	3.728%
8	9.186	1203	1207	1217	rBV	3364330	3211309	100.00%	9.439%
9	9.581	1270	1274	1283	rBV	417464	399187	12.43%	1.173%
10	9.863	1319	1322	1333	rBV	1359621	1375799	42.84%	4.044%
11	10.657	1453	1457	1472	rBV	1957912	1999827	62.27%	5.878%
12	10.763	1472	1475	1480	rVB	37183	39728	1.24%	0.117%
13	11.351	1572	1575	1585	rBV	1404271	1430893	44.56%	4.206%
14	11.875	1660	1664	1677	rBV2	251732	346962	10.80%	1.020%
15	12.657	1795	1797	1802	rBV4	24970	35488	1.11%	0.104%
16	12.933	1839	1844	1847	rBV	2894590	2693885	83.89%	7.918%
17	13.851	1992	2000	2006	rBV4	155913	441430	13.75%	1.298%
18	13.957	2016	2018	2021	rBV	53193	34600	1.08%	0.102%
19	13.998	2021	2025	2031	rVB	1031732	1035532	32.25%	3.044%
20	14.139	2046	2049	2053	rBV	123098	125257	3.90%	0.368%
21	14.445	2097	2101	2104	rBV	317311	298395	9.29%	0.877%
22	14.745	2148	2152	2157	rBV	601157	626206	19.50%	1.841%
23	15.080	2204	2209	2215	rVB	764291	914500	28.48%	2.688%
24	15.457	2267	2273	2285	rBV2	1099021	2013404	62.70%	5.918%
25	15.880	2340	2345	2356	rVB	500136	853832	26.59%	2.510%
26	16.374	2423	2429	2439	rVB	225451	468746	14.60%	1.378%

Sum of corrected areas: 34021508

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052219\
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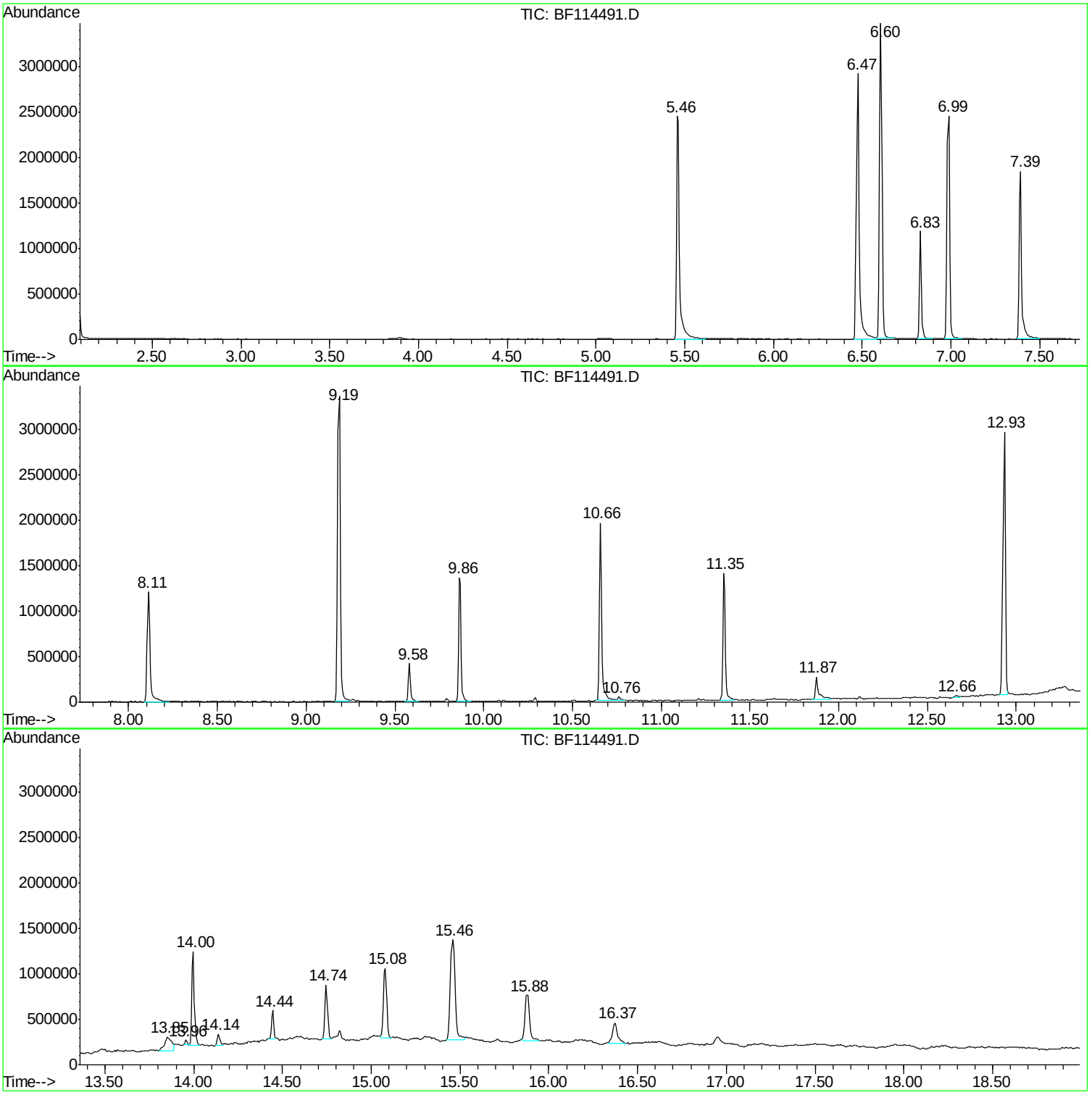
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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\BF052219\
Data File : BF114491.D
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Instrument : BNA_F
ClientSampleId : DB-4

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

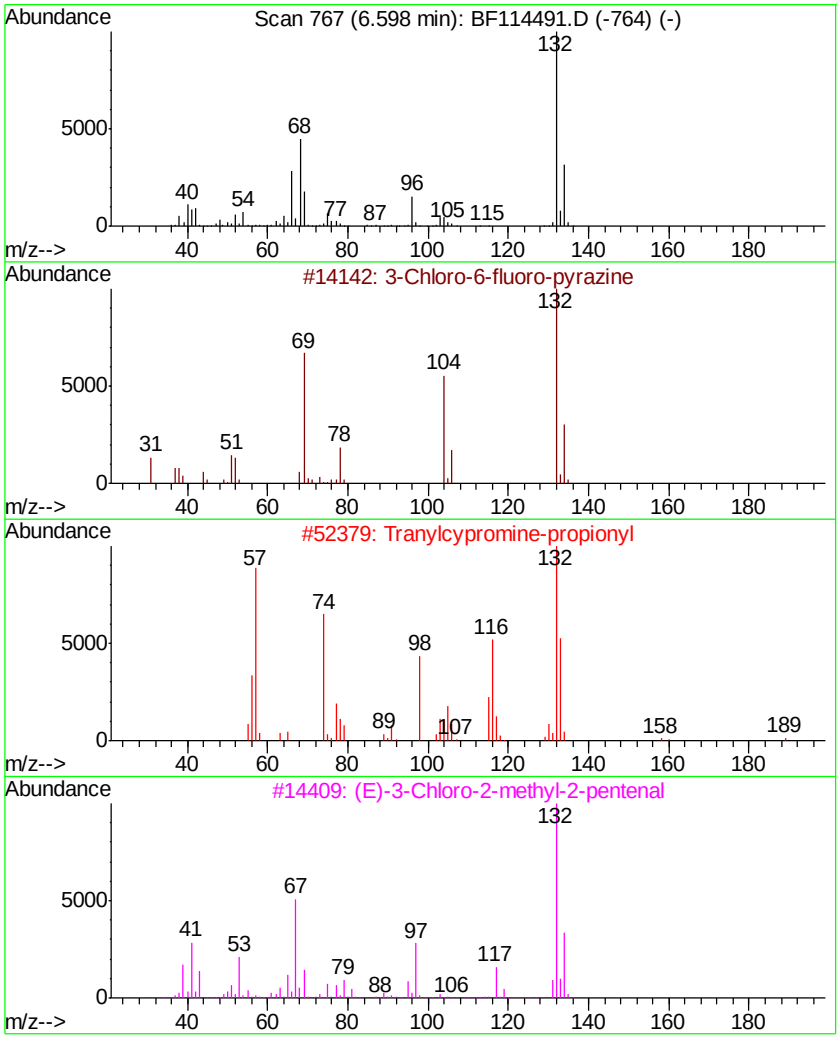
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

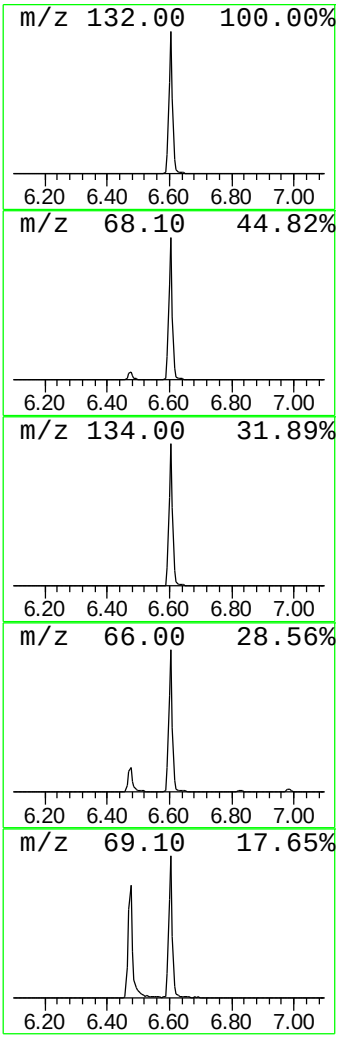
****

Peak Number 1 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	62.42 ng	3029750	1,4-Dichlorobenzene-d4	6.83

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	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Data File : BF114491.D
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Operator : JU/SJ
Sample : K2962-10
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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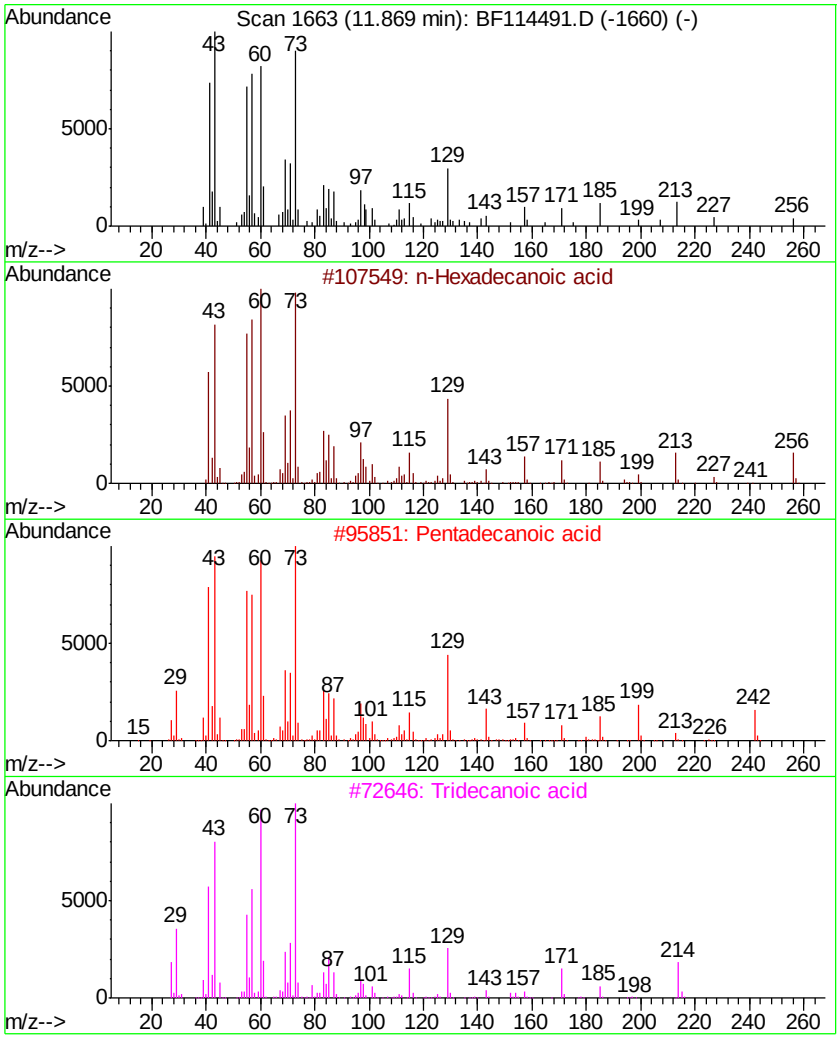
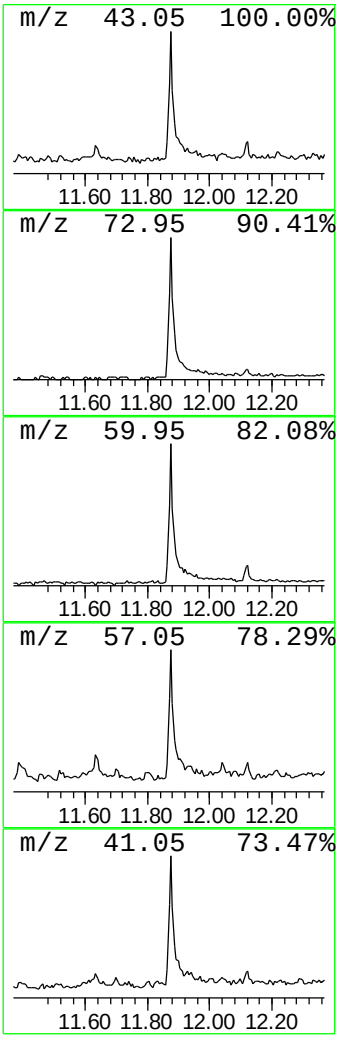
Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	4.85 ng	346962	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052219\
Data File : BF114491.D
Acq On : 22 May 2019 19:01
Operator : JU/SJ
Sample : K2962-10
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

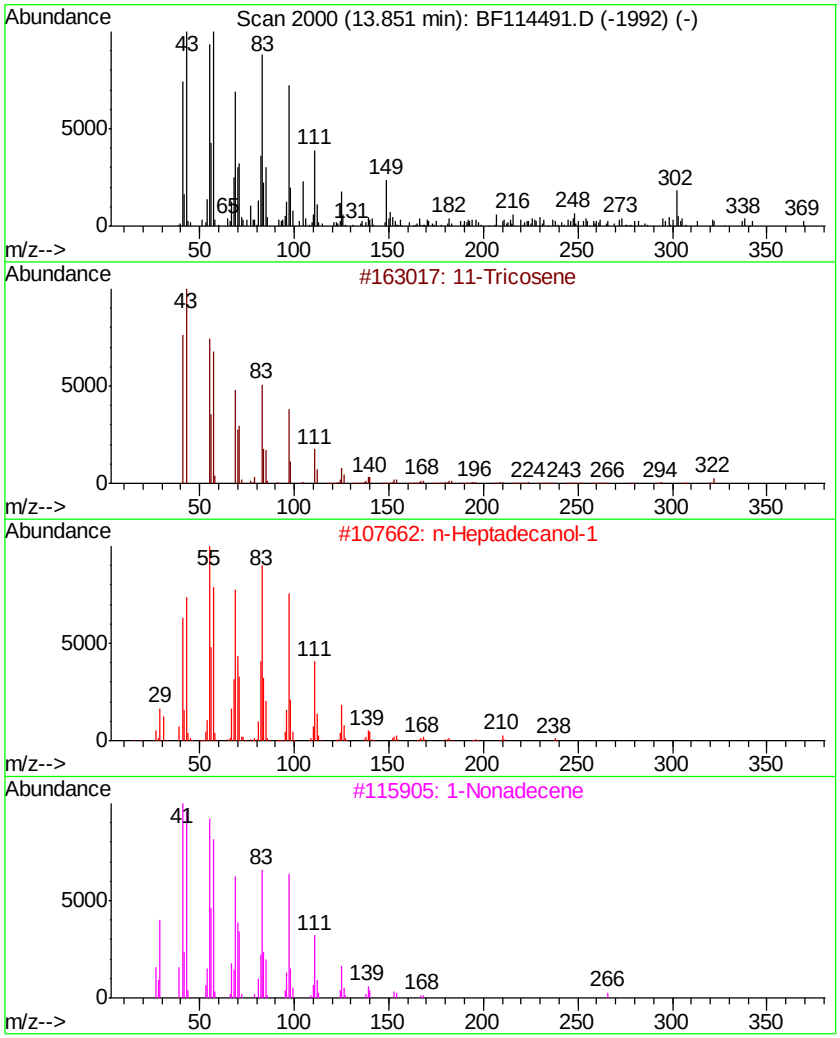
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

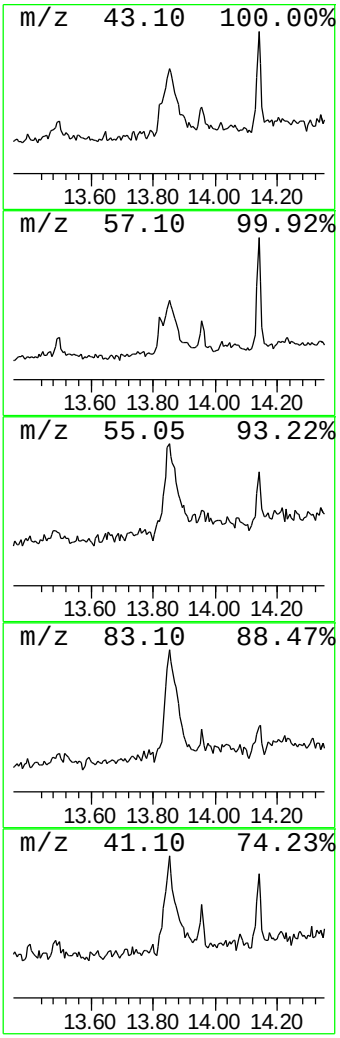
****

Peak Number 4 11-Tricosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	8.53 ng	441430	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Tricosene	322	C23H46	052078-56-5	93
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	93
3	1-Nonadecene	266	C19H38	018435-45-5	92
4	9-Tricosene, (Z)-	322	C23H46	027519-02-4	91
5	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052219\
Data File : BF114491.D
Acq On : 22 May 2019 19:01
Operator : JU/SJ
Sample : K2962-10
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

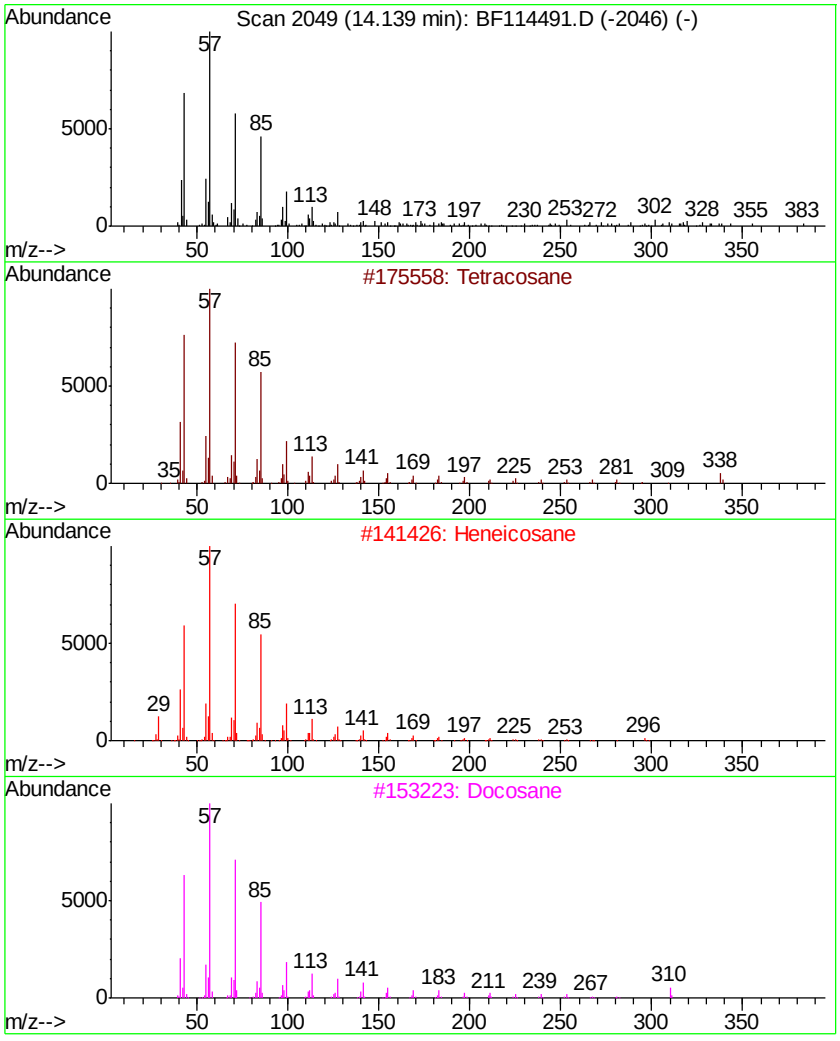
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

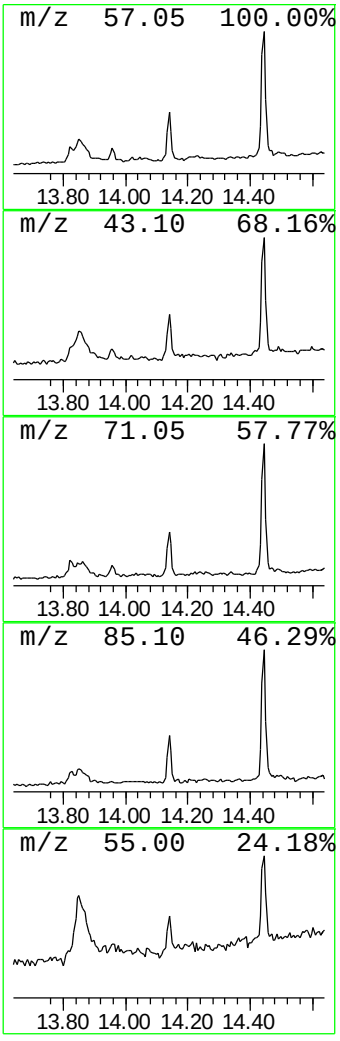
****

Peak Number 5 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	2.42 ng	125257	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	93
2	Heneicosane	296	C21H44	000629-94-7	93
3	Docosane	310	C22H46	000629-97-0	87
4	Tricosane, 2-methyl-	338	C24H50	001928-30-9	87
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052219\
Data File : BF114491.D
Acq On : 22 May 2019 19:01
Operator : JU/SJ
Sample : K2962-10
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

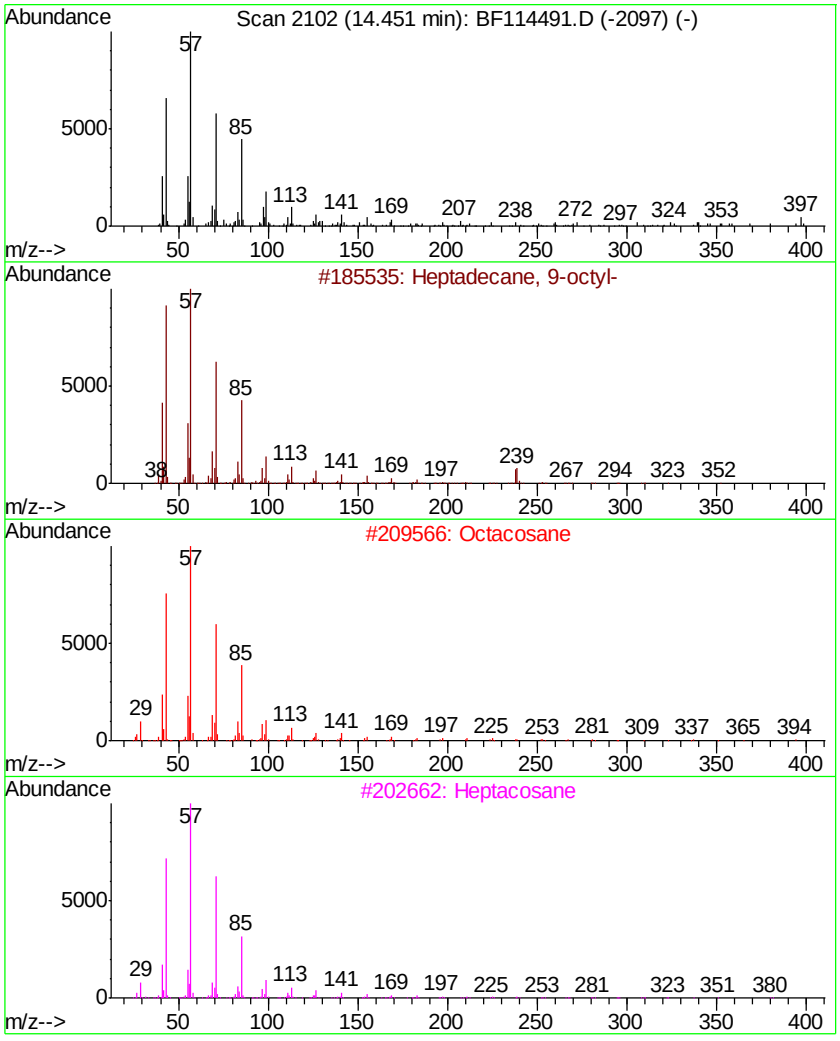
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

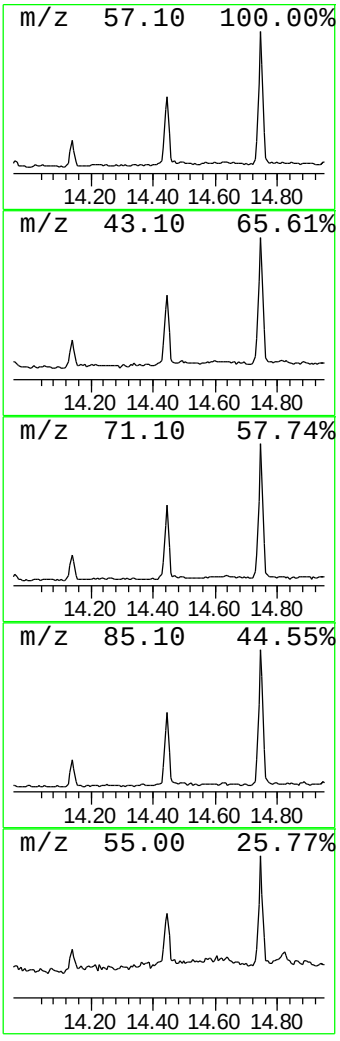
****

Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	5.76 ng	298395	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
2	Octacosane	394	C28H58	000630-02-4	90
3	Heptacosane	380	C27H56	000593-49-7	90
4	Heneicosane	296	C21H44	000629-94-7	87
5	Pentadecane	212	C15H32	000629-62-9	87





Library Search Compound Report

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Acq On : 22 May 2019 19:01
Operator : JU/SJ
Sample : K2962-10
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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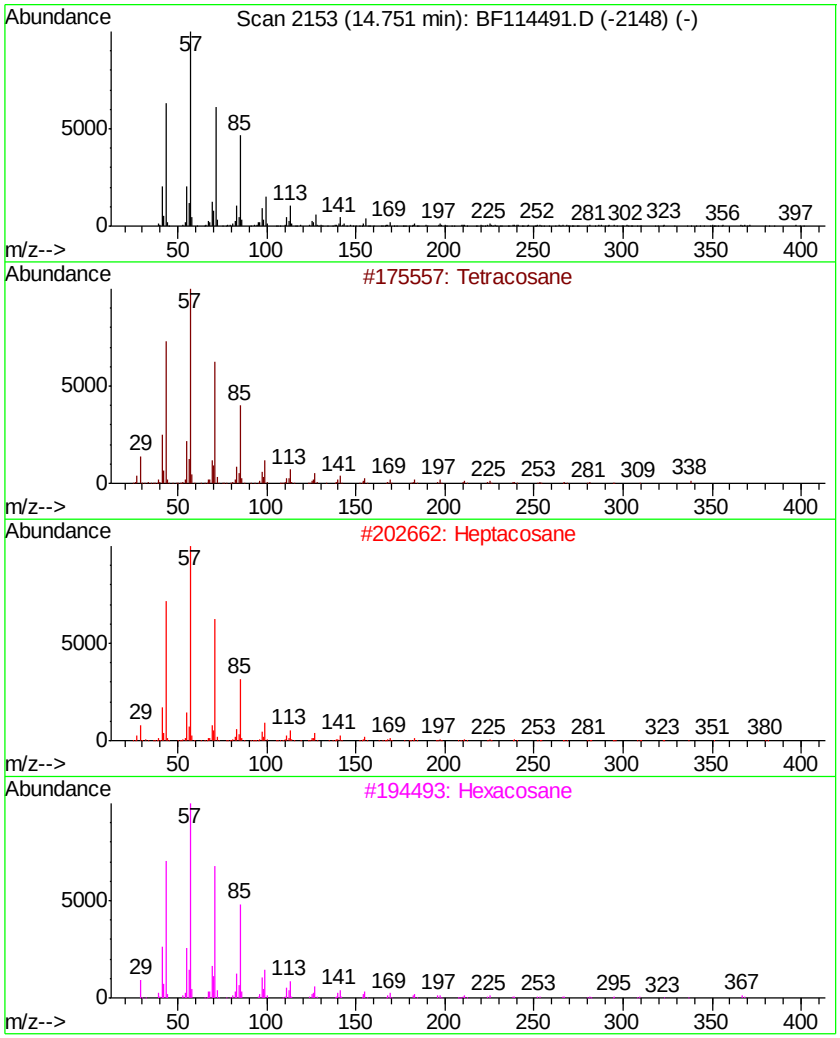
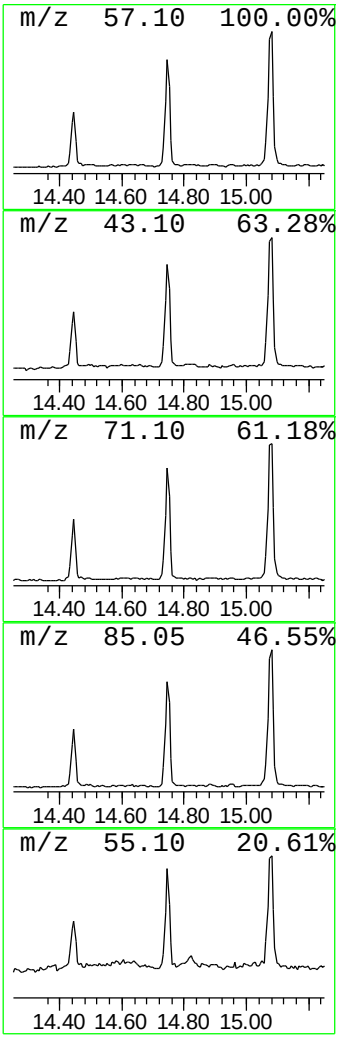
Peak Number 7 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	6.22 ng	626206	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	94
2	Heptacosane	380	C27H56	000593-49-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	Triacontane	422	C30H62	000638-68-6	91





Library Search Compound Report

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Sample : K2962-10
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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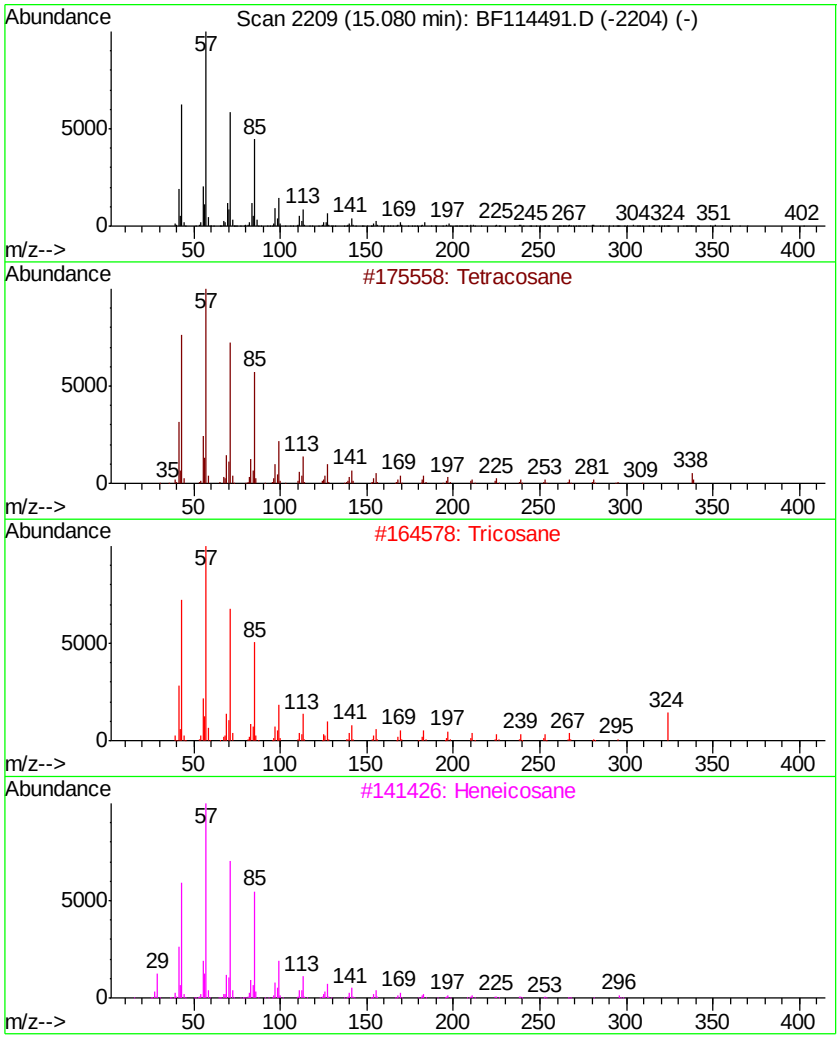
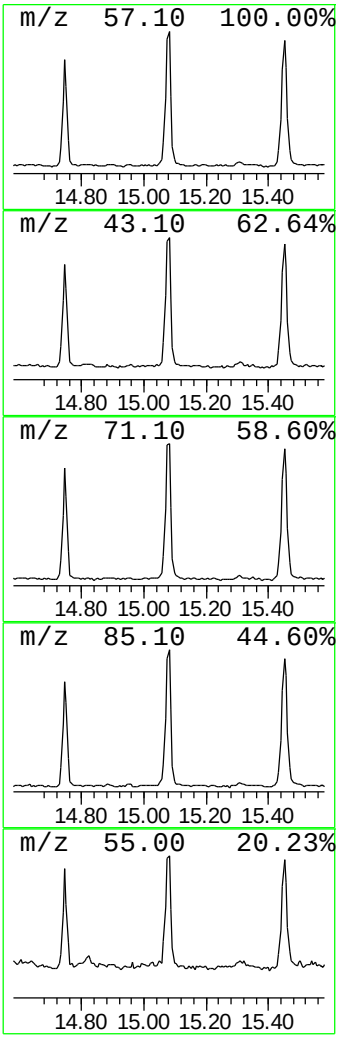
Peak Number 8 Tricosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	9.08 ng	914500	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	94
2	Tricosane	324	C23H48	000638-67-5	93
3	Heneicosane	296	C21H44	000629-94-7	91
4	Docosane	310	C22H46	000629-97-0	91
5	Heptacosane	380	C27H56	000593-49-7	91





Library Search Compound Report

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Operator : JU/SJ
Sample : K2962-10
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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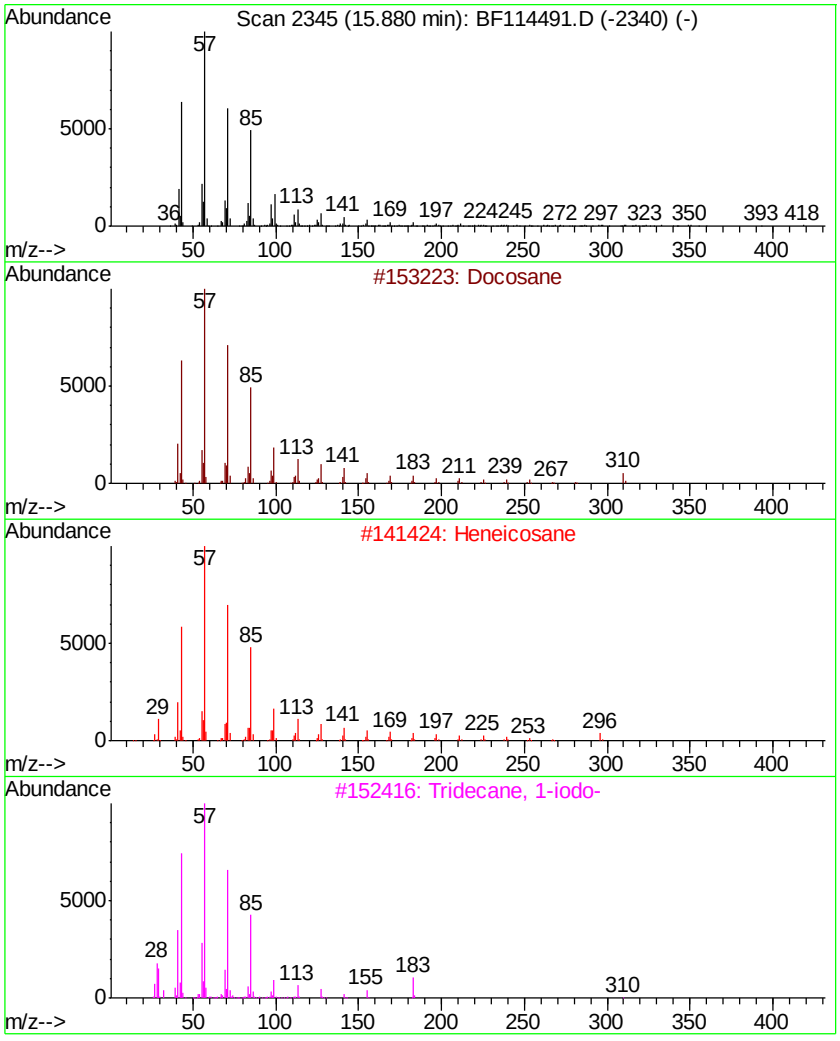
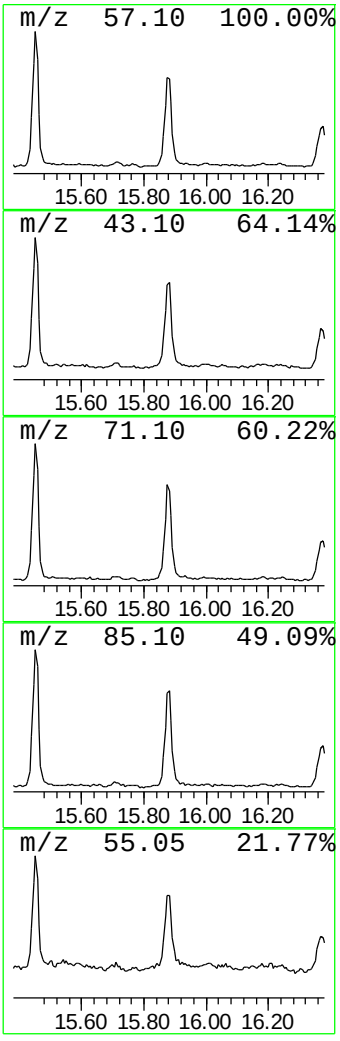
Peak Number 9 Docosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	8.48 ng	853832	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	93
2	Heneicosane	296	C21H44	000629-94-7	93
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	93
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Octacosane	394	C28H58	000630-02-4	91





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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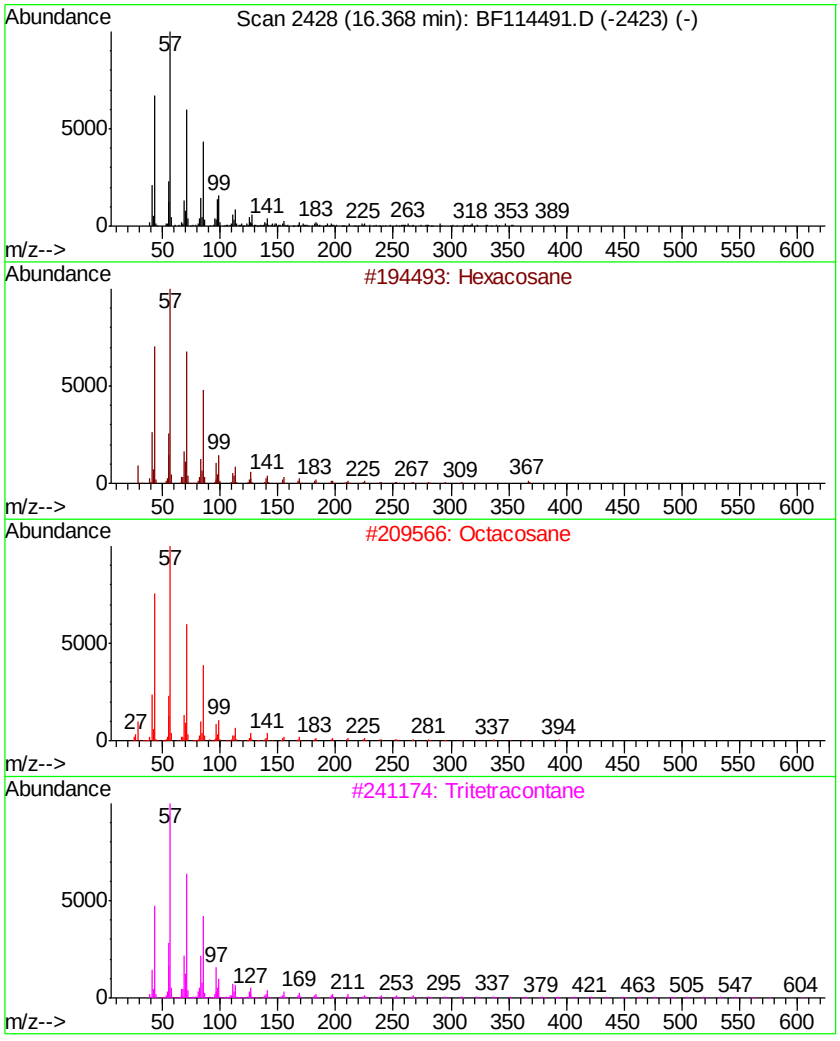
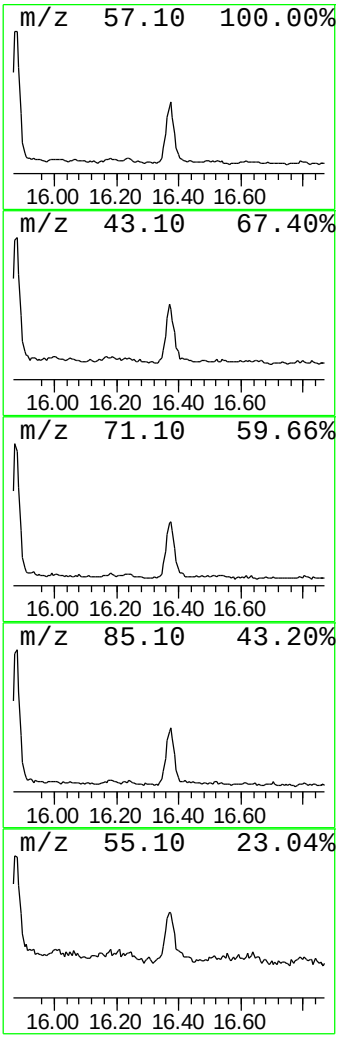
Peak Number 10 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.37	4.66 ng	468746	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Octacosane	394	C28H58	000630-02-4	90
3	Tritetracontane	605	C43H88	007098-21-7	90
4	Hexatriacontane	507	C36H74	000630-06-8	87
5	Tricosane, 2-methyl-	338	C24H50	001928-30-9	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF052219\
Data File : BF114491.D
Acq On : 22 May 2019 19:01
Operator : JU/SJ
Sample : K2962-10
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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
unknown6.60	6.60	62.4	ng	3029750	1	6.83	970775	20.0
n-Hexadecanoic acid	11.87	4.8	ng	346962	4	11.35	1430890	20.0
11-Tricosene	13.85	8.5	ng	441430	5	14.00	1035530	20.0
Tetracosane	14.14	2.4	ng	125257	5	14.00	1035530	20.0
Heptadecane, 9-oc...	14.45	5.8	ng	298395	5	14.00	1035530	20.0
Heptacosane	14.75	6.2	ng	626206	6	15.46	2013400	20.0
Tricosane	15.08	9.1	ng	914500	6	15.46	2013400	20.0
Docosane	15.88	8.5	ng	853832	6	15.46	2013400	20.0
Hexacosane	16.37	4.7	ng	468746	6	15.46	2013400	20.0