LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051119\
Data File : BF114170.D
Acq On : 11 May 2019 23:07
Operator : JU/SJ
Sample : K2765-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS004-0612-01

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	2.116	3	5	21	rVB	1403675	1546551	20.28%	2.003%
2	5.481	572	577	580	rBV	6440910	6530742	85.63%	8.459%
3	6.487	743	748	751	rBV	6800260	7490597	98.21%	9.703%
4	6.622	767	771	775	rBV	7168662	7114457	93.28%	9.215%
5	6.851	806	810	813	rBV	1965256	1673912	21.95%	2.168%
6	7.010	832	837	840	rBV	5746816	5366437	70.36%	6.951%
7	7.410	900	905	908	rBV	5103215	4684331	61.42%	6.068%
8	8.128	1023	1027	1031	rBV	2530691	2111986	27.69%	2.736%
9	9.204	1205	1210	1213	rBV	8453798	7626993	100.00%	9.879%
10	9.592	1273	1276	1281	rBV	1353448	1061781	13.92%	1.375%
11	9.880	1321	1325	1329	rBV	2825505	2321146	30.43%	3.007%
12	10.669	1455	1459	1463	rBV	5021092	5022835	65.86%	6.506%
13	11.363	1573	1577	1580	rBV	2760714	2582435	33.86%	3.345%
14	11.386	1580	1581	1587	rVB	314161	224135	2.94%	0.290%
15	11.816	1651	1654	1660	rBV3	72584	94930	1.24%	0.123%
16	11.863	1660	1662	1664	rBV	90223	82386	1.08%	0.107%
17	11.892	1664	1667	1678	rVB	1445460	1525357	20.00%	1.976%
18	11.998	1683	1685	1689	rVB	83290	84854	1.11%	0.110%
19	12.186	1714	1717	1721	rVB2	90218	81375	1.07%	0.105%
20	12.416	1751	1756	1759	rBV4	91212	121602	1.59%	0.158%
21	12.498	1767	1770	1775	rBV	80556	81712	1.07%	0.106%
22	12.574	1780	1783	1786	rBV	416491	357213	4.68%	0.463%
23	12.674	1797	1800	1803	rBV2	401215	369004	4.84%	0.478%
24	12.804	1818	1822	1825	rBV	710055	617720	8.10%	0.800%
25	12.951	1842	1847	1850	rBV	7735167	7527777	98.70%	9.751%
26	13.021	1856	1859	1866	rBV2	75551	104339	1.37%	0.135%
27	13.110	1871	1874	1876	rBV3	70779	86003	1.13%	0.111%
28	13.327	1908	1911	1914	rBV	98120	104540	1.37%	0.135%
29	13.639	1961	1964	1968	rVB	89335	83671	1.10%	0.108%
30	13.839	1994	1998	2006	rBV2	1322431	1580955	20.73%	2.048%
31	13.998	2020	2025	2028	rBV	2065660	2244713	29.43%	2.908%
32	14.027	2028	2030	2036	rVB	250052	229902	3.01%	0.298%
33	14.163	2051	2053	2062	rVB3	182836	256243	3.36%	0.332%
34	14.468	2101	2105	2110	rBV	259737	311350	4.08%	0.403%

LSC Area Percent Report

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Operator : JU/SJ
Sample : K2765-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS004-0612-01

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

35	14.751	2150	2153	2155	rBV	209425	205100	2.69%	0.266%
36	14.774	2155	2157	2160	rVB	255261	216320	2.84%	0.280%
37	14.851	2166	2170	2174	rBV	972775	950833	12.47%	1.232%
38	15.033	2198	2201	2210	rVB2	219540	433260	5.68%	0.561%
39	15.110	2210	2214	2217	rBV	281796	304167	3.99%	0.394%
40	15.339	2249	2253	2259	rVV	155908	210171	2.76%	0.272%
41	15.398	2259	2263	2268	rVV	169557	193764	2.54%	0.251%
42	15.462	2269	2274	2288	rVB	1586574	2334841	30.61%	3.024%
43	15.921	2346	2352	2356	rBV	183051	281634	3.69%	0.365%
44	15.968	2356	2360	2367	rBV3	112123	240627	3.15%	0.312%
45	16.421	2432	2437	2442	rVB2	86489	145826	1.91%	0.189%
46	16.915	2516	2521	2527	rBV2	88209	162522	2.13%	0.211%
47	17.351	2592	2595	2604	rVB	107965	219003	2.87%	0.284%

Sum of corrected areas: 77202052

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051119\
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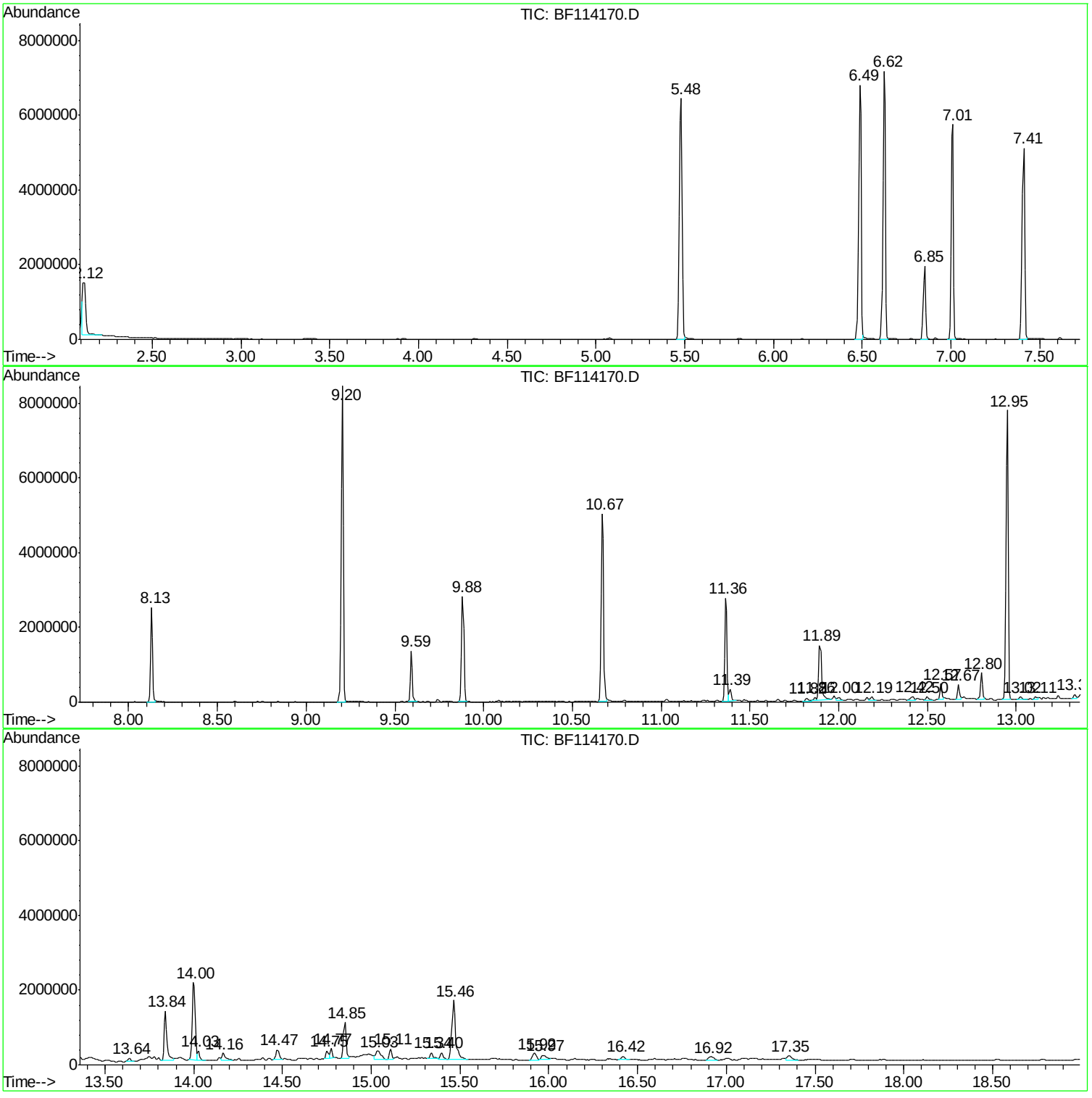
Acq On : 11 May 2019 23:07
Operator : JU/SJ
Sample : K2765-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS004-0612-01

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\BF051119\
Data File : BF114170.D
Acq On : 11 May 2019 23:07
Operator : JU/SJ
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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS004-0612-01

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

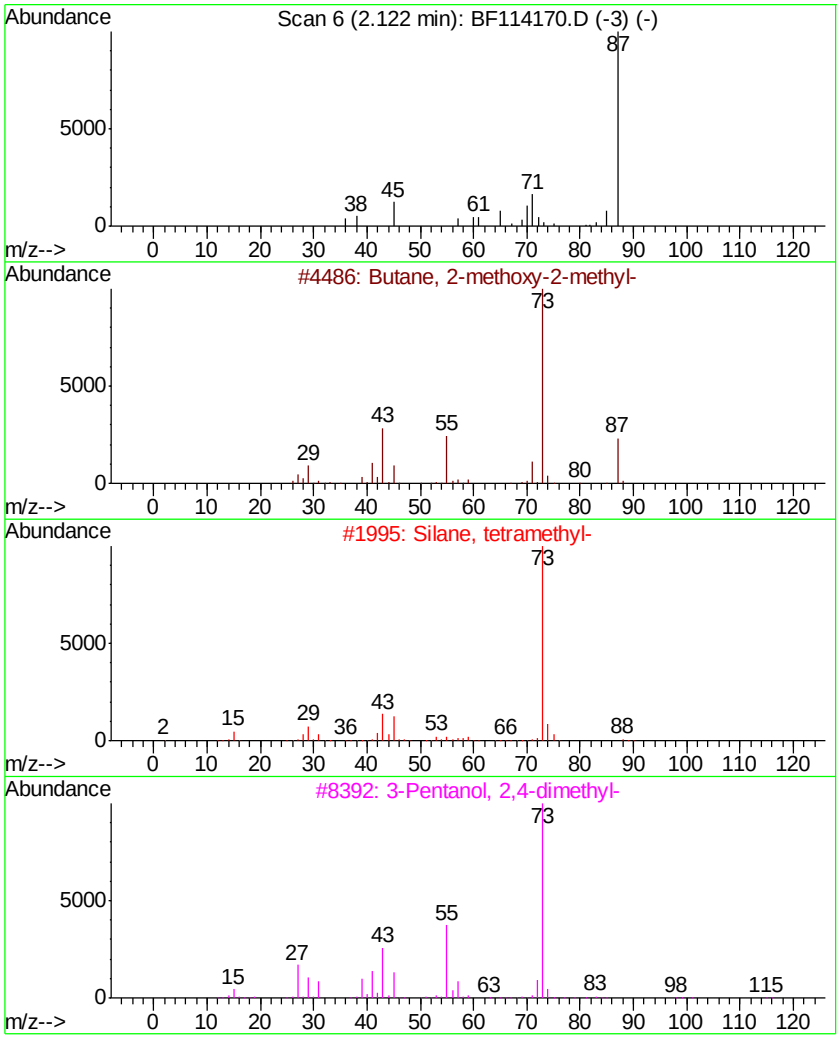
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

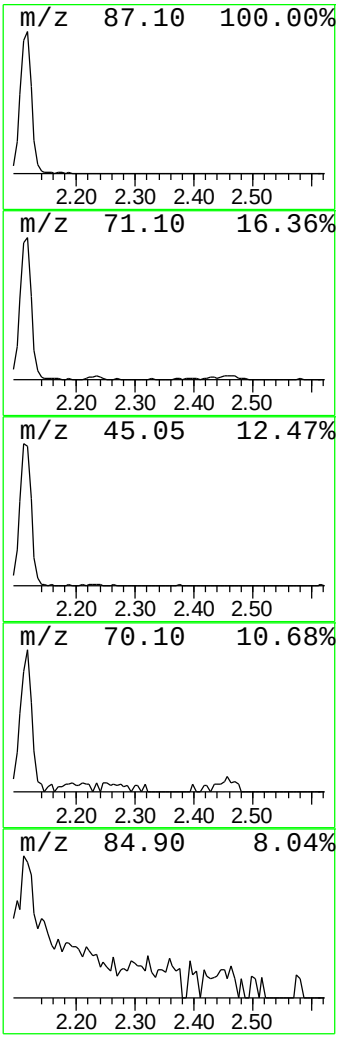
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	18.48 ng	1546550	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	56
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	32
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





Library Search Compound Report

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Operator : JU/SJ
Sample : K2765-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS004-0612-01

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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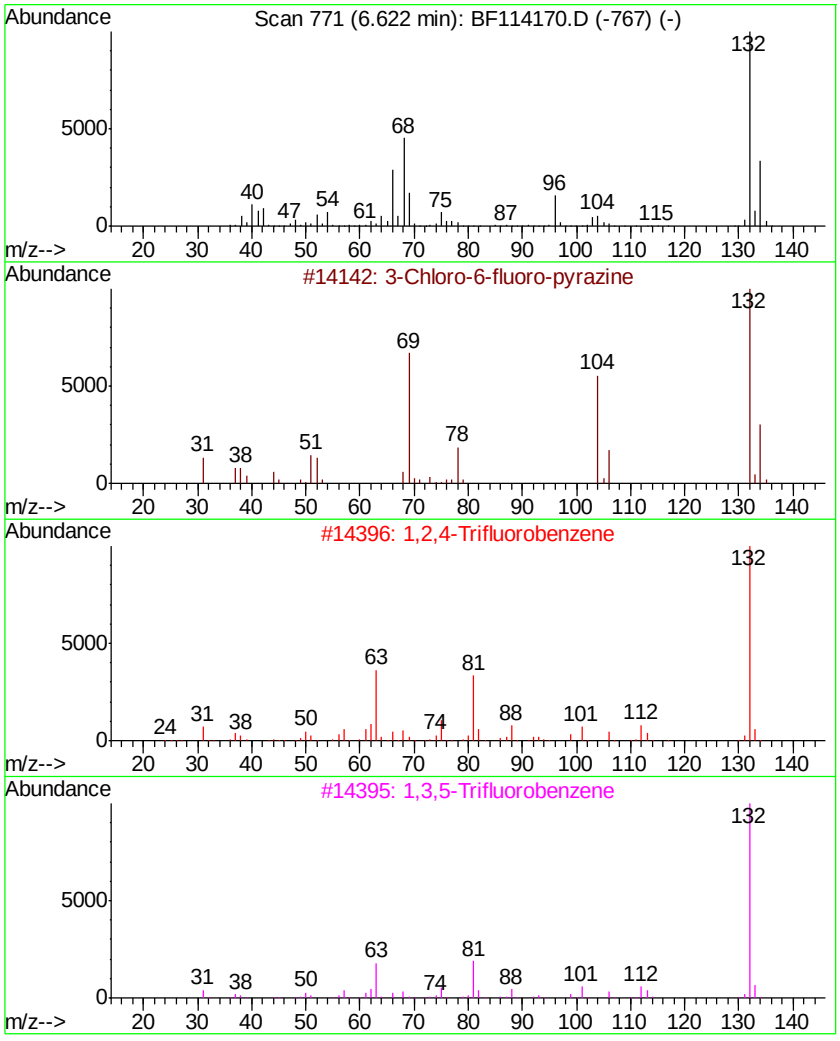
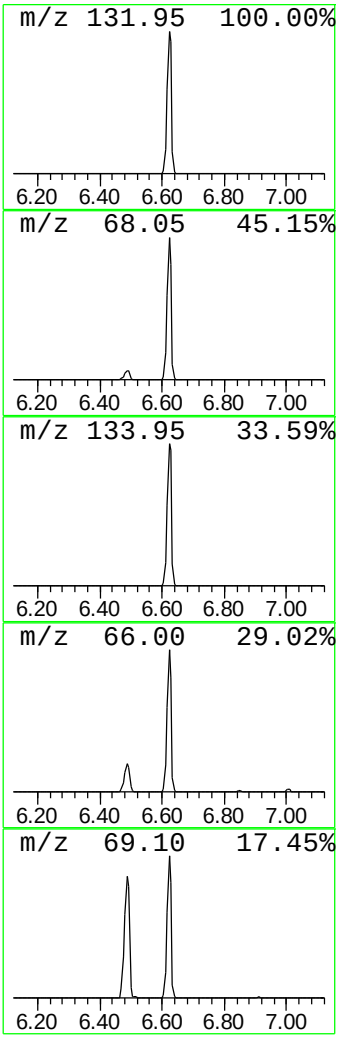
Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	85.00 ng	7114460	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	27
2	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	Xenon	132	Xe	007440-63-3	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 : BF114170.D
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Operator : JU/SJ
Sample : K2765-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS004-0612-01

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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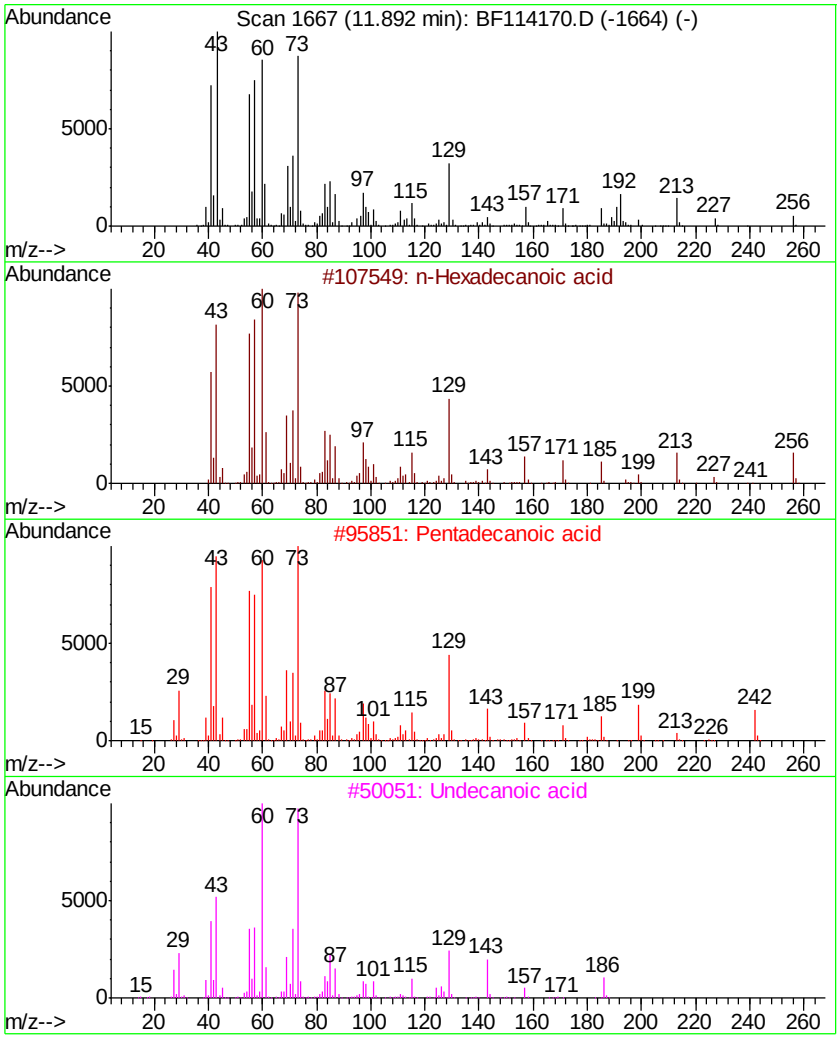
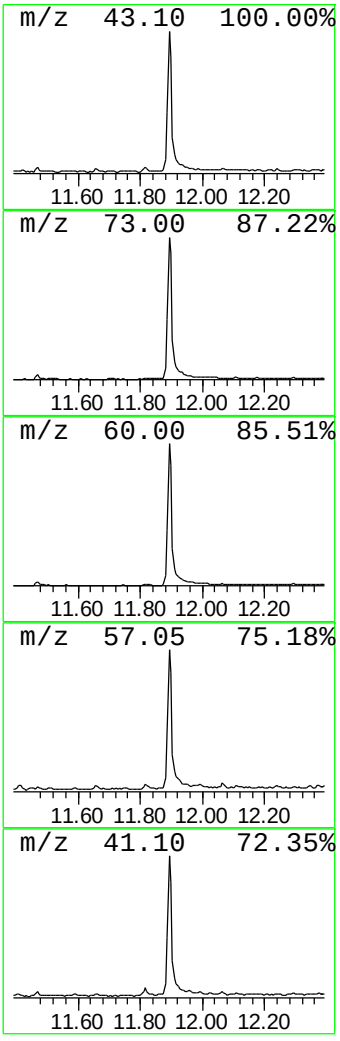
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	11.81 ng	1525360	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Undecanoic acid	186	C11H22O2	000112-37-8	62
4	n-Decanoic acid	172	C10H20O2	000334-48-5	60
5	Tridecanoic acid	214	C13H26O2	000638-53-9	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051119\
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Operator : JU/SJ
Sample : K2765-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS004-0612-01

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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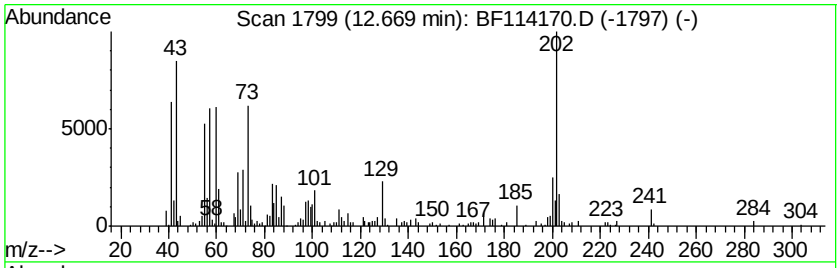
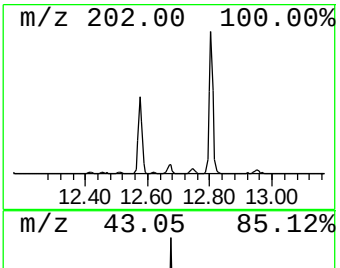
Peak Number 5 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	2.86 ng	369004	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	68
5	Tridecanoic acid	214	C13H26O2	000638-53-9	62





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Operator : JU/SJ
Sample : K2765-10
Misc :
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Instrument : BNA_F
ClientSampleId : P026-SS004-0612-01

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
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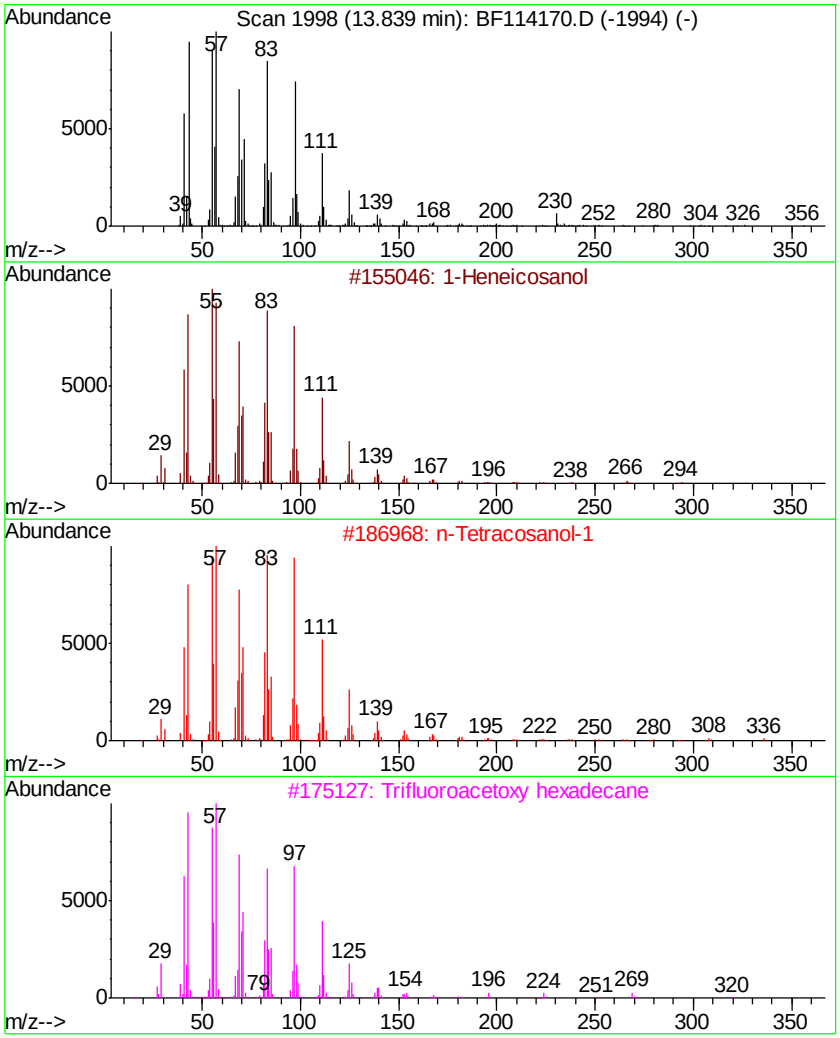
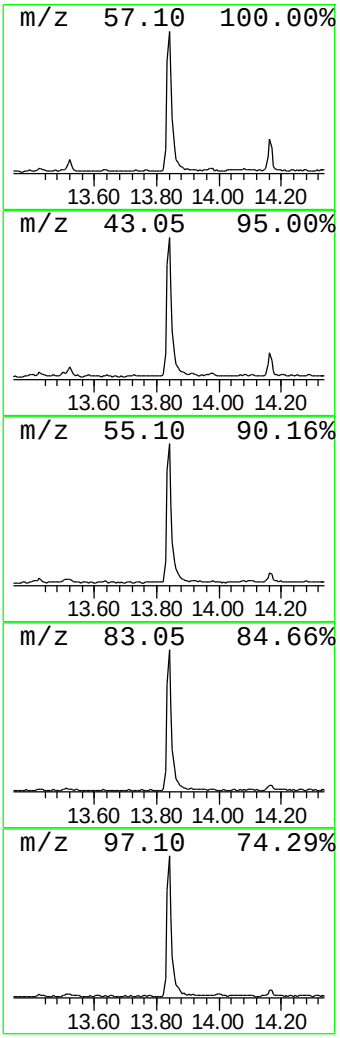
****

Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	14.09 ng	1580960	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5	10-Heneicosene (c,t)	294	C21H42	095008-11-0	91





Library Search Compound Report

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ClientSampleId : P026-SS004-0612-01

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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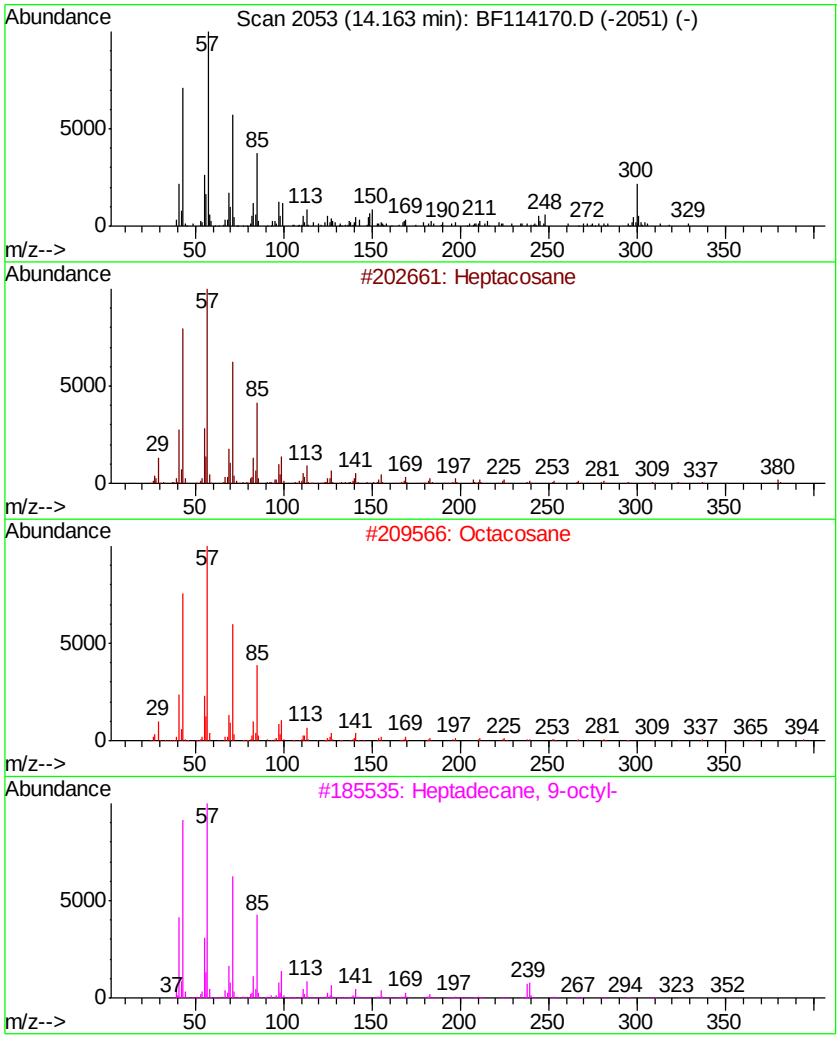
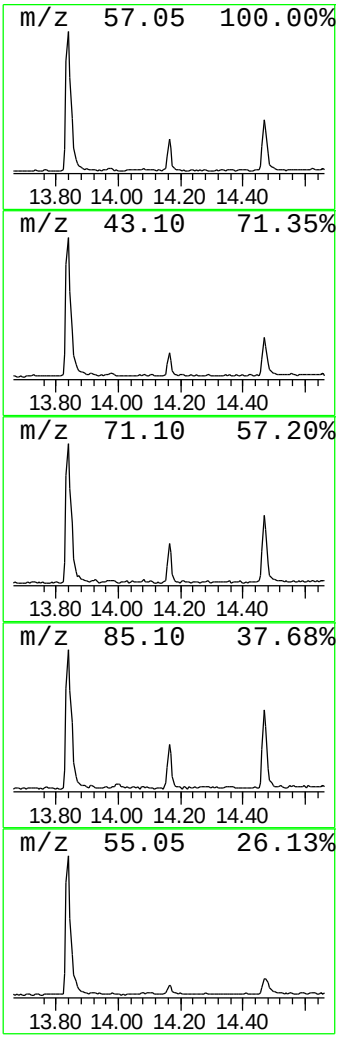
Peak Number 7 Heptacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.16	2.28 ng	256243	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	70
2	Octacosane	394	C28H58	000630-02-4	70
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	62
4	Hexatriacontane	507	C36H74	000630-06-8	62
5	Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	62





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS004-0612-01

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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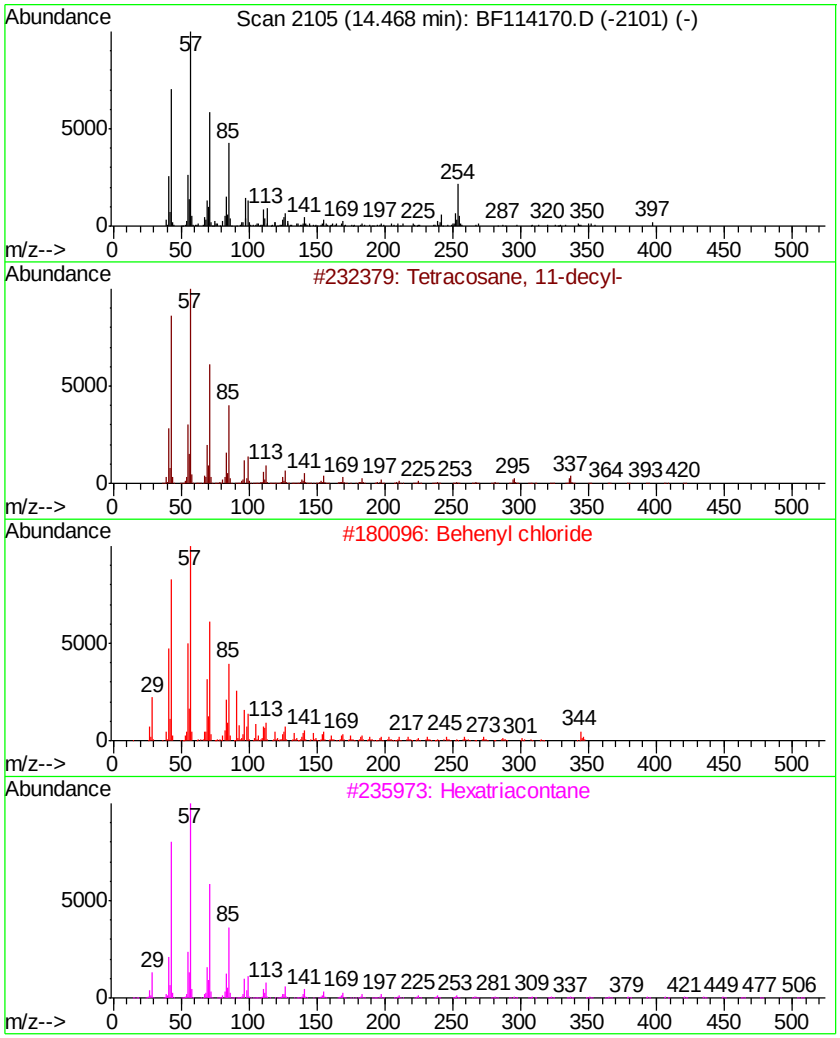
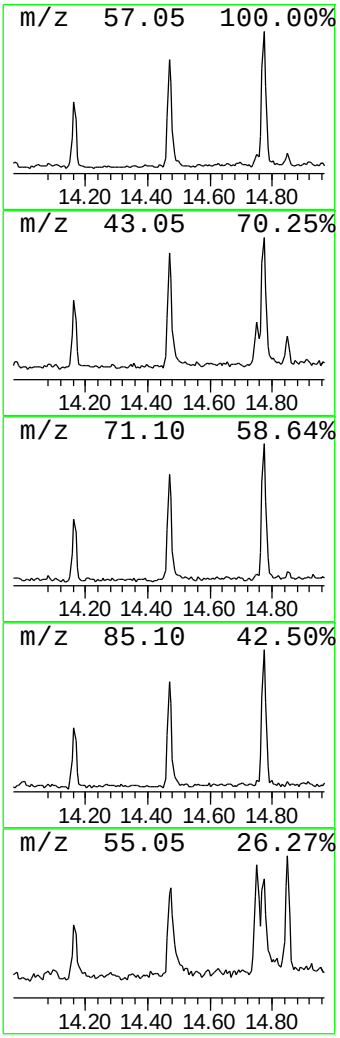
Peak Number 8 Tetracosane, 11-decyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	2.77 ng	311350	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	76
2	Behenyl chloride	344	C22H45Cl	042217-03-8	76
3	Hexatriacontane	507	C36H74	000630-06-8	76
4	Tetracosane	338	C24H50	000646-31-1	70
5	Heptacosane	380	C27H56	000593-49-7	68





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051119\
Data File : BF114170.D
Acq On : 11 May 2019 23:07
Operator : JU/SJ
Sample : K2765-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS004-0612-01

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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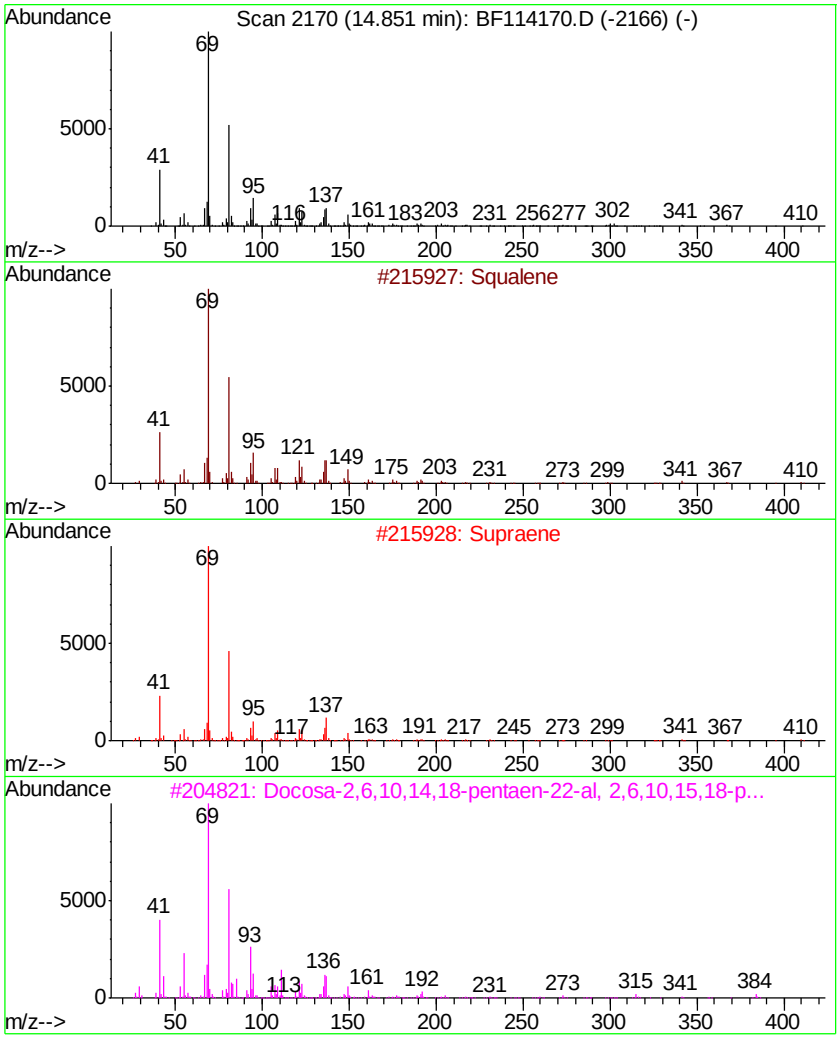
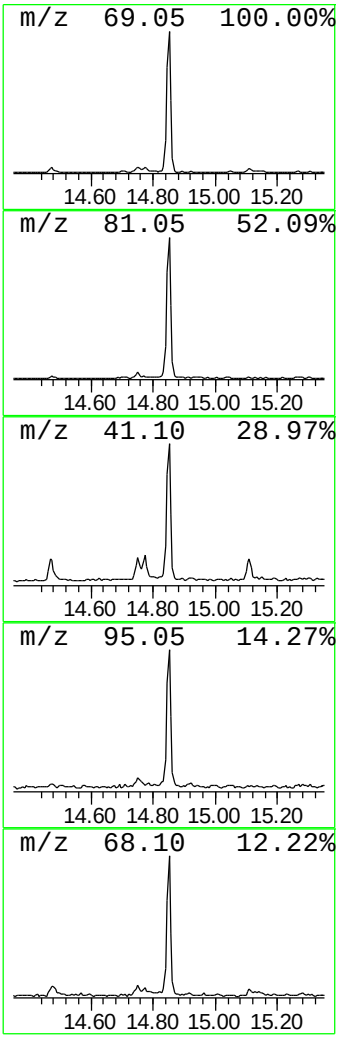
Peak Number 9 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	8.14 ng	950833	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	94
2	Supraene	410	C30H50	007683-64-9	91
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4	2,6,10,14-Hexadecatetraenoic aci...	318	C21H34O2	042207-88-5	72
5	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051119\
Data File : BF114170.D
Acq On : 11 May 2019 23:07
Operator : JU/SJ
Sample : K2765-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS004-0612-01

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

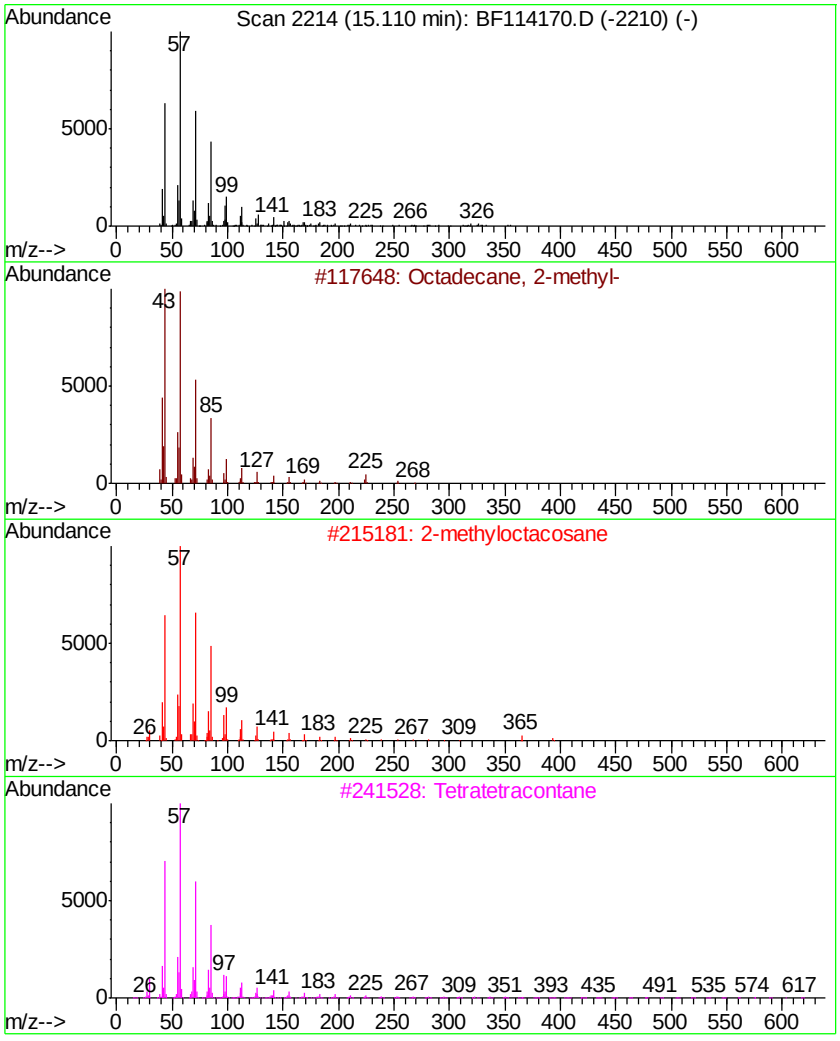
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

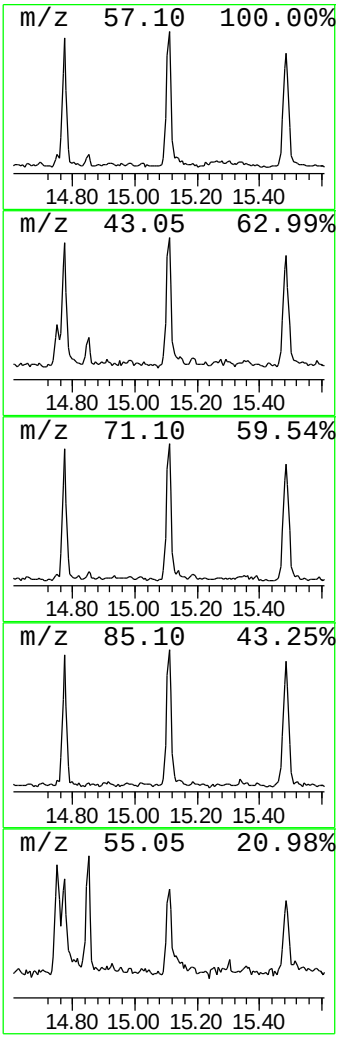
****

Peak Number 11 Octadecane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.11	2.61 ng	304167	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Library Search Compound Report

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Data File : BF114170.D
Acq On : 11 May 2019 23:07
Operator : JU/SJ
Sample : K2765-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS004-0612-01

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

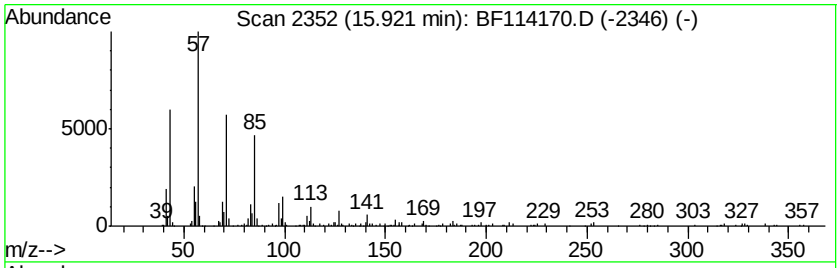
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

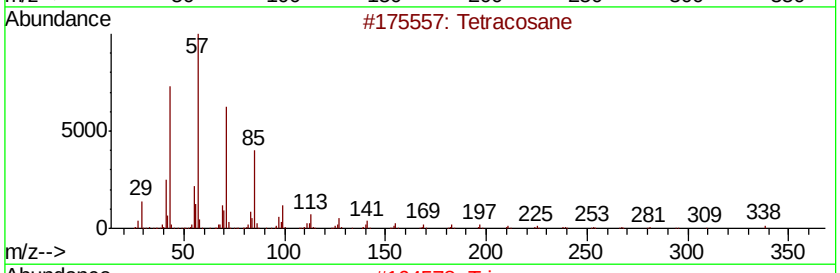
****

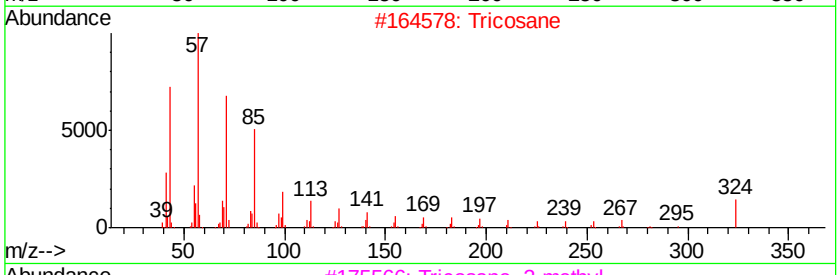
Peak Number 12 Tetracosane Concentration Rank 11

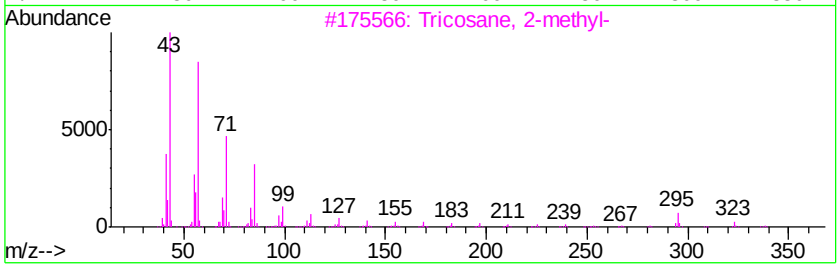
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	2.41 ng	281634	Perylene-d12	15.46

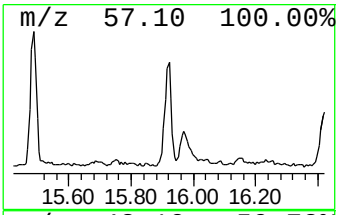
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	97
2	Tricosane	324	C23H48	000638-67-5	96
3	Tricosane, 2-methyl-	338	C24H50	001928-30-9	94
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Heneicosane	296	C21H44	000629-94-7	90

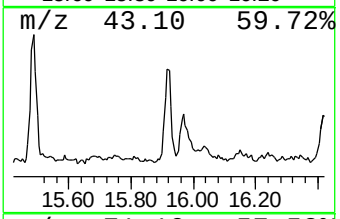


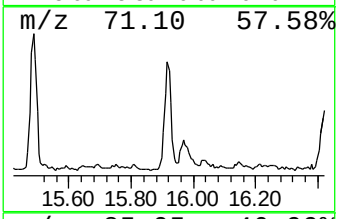


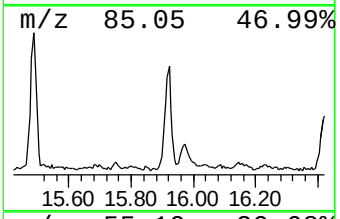


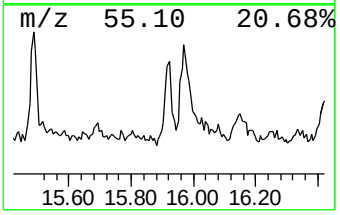












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Instrument : BNA_F
ClientSampleId : P026-SS004-0612-01

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

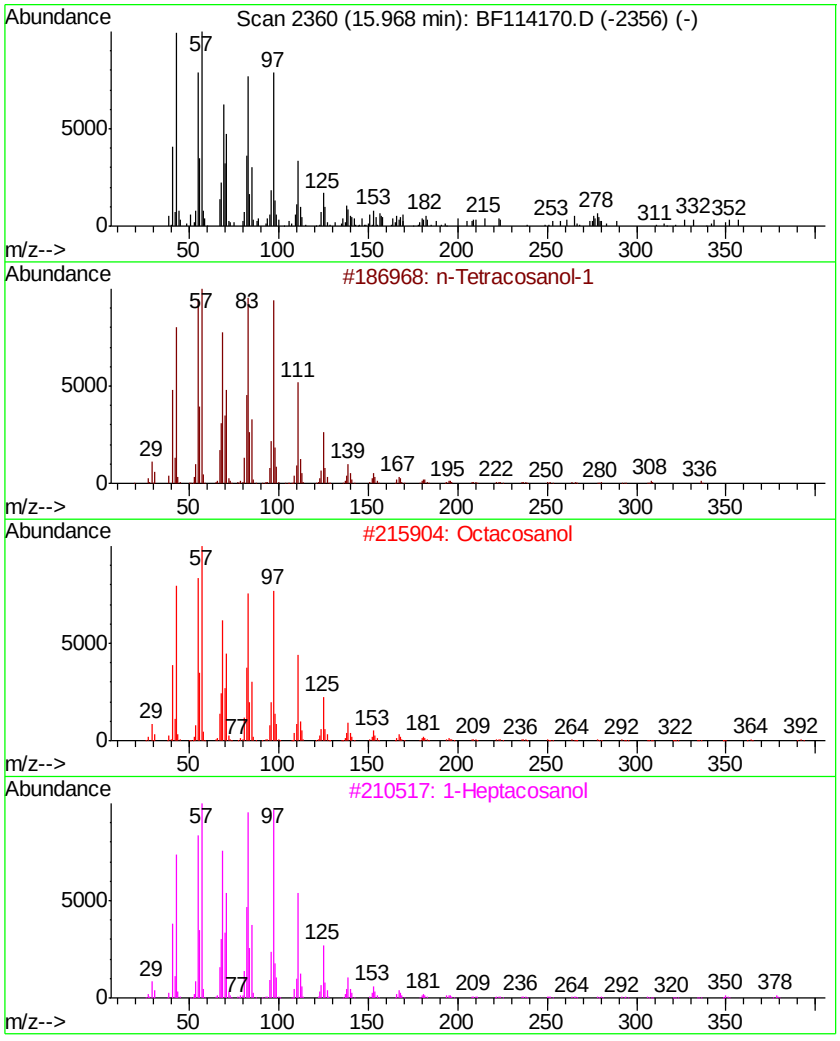
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

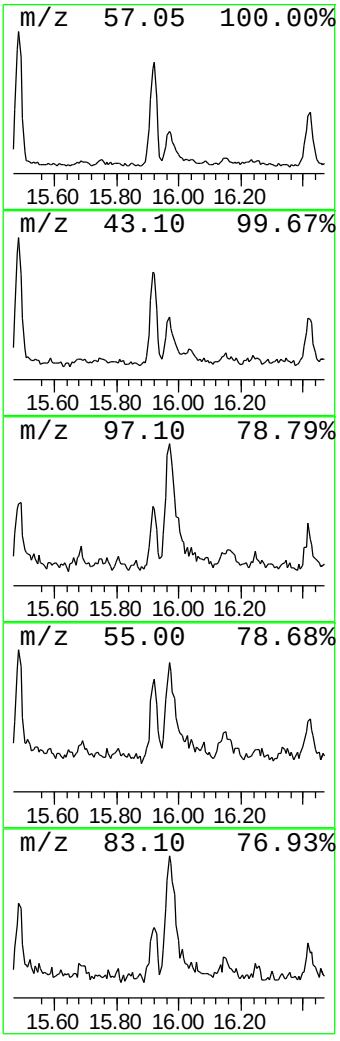
****

Peak Number 13 n-Tetracosanol-1 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	2.06 ng	240627	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
2	Octacosanol	410	C28H58O	000557-61-9	93
3	1-Heptacosanol	396	C27H56O	002004-39-9	93
4	Heptacosyl acetate	438	C29H58O2	1000351-78-2	93
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051119\
Data File : BF114170.D
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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...	2.12	18.5	ng	1546550	1	6.85	1673910	20.0
unknown6.62	6.62	85.0	ng	7114460	1	6.85	1673910	20.0
n-Hexadecanoic acid	11.89	11.8	ng	1525360	4	11.36	2582440	20.0
Octadecanoic acid	12.67	2.9	ng	369004	4	11.36	2582440	20.0
1-Heneicosanol	13.84	14.1	ng	1580960	5	14.00	2244710	20.0
Heptacosane	14.16	2.3	ng	256243	5	14.00	2244710	20.0
Tetracosane, 11-d...	14.47	2.8	ng	311350	5	14.00	2244710	20.0
Squalene	14.85	8.1	ng	950833	6	15.46	2334840	20.0
Octadecane, 2-met...	15.11	2.6	ng	304167	6	15.46	2334840	20.0
Tetracosane	15.92	2.4	ng	281634	6	15.46	2334840	20.0
n-Tetracosanol-1	15.97	2.1	ng	240627	6	15.46	2334840	20.0