LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052419\
Data File : BF114575.D
Acq On : 24 May 2019 17:52
Operator : JU/SJ
Sample : K2993-16
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

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	5.028	496	500	514	rBV	1222832	1612517	35.55%	3.267%
2	5.451	569	572	597	rBV	3241550	3442459	75.89%	6.974%
3	6.469	740	745	762	rBV	3623421	4123140	90.89%	8.353%
4	6.592	762	766	779	rVB	4109867	3757558	82.83%	7.612%
5	6.810	800	803	811	rBV	1123377	962434	21.22%	1.950%
6	6.969	826	830	846	rBV	3580007	3168321	69.84%	6.418%
7	7.375	895	899	911	rBV	2737818	2670277	58.86%	5.409%
8	8.092	1017	1021	1036	rBV	1370149	1246871	27.49%	2.526%
9	9.169	1199	1204	1207	rBV	5057277	4479116	98.74%	9.074%
10	9.563	1268	1271	1275	rBV	273846	239395	5.28%	0.485%
11	9.845	1315	1319	1325	rBV2	1452811	1384135	30.51%	2.804%
12	10.639	1451	1454	1462	rBV	1802084	1991355	43.90%	4.034%
13	11.268	1546	1561	1569	rBV9	237750	1327042	29.25%	2.688%
14	11.333	1569	1572	1579	rVB	1547397	1570114	34.61%	3.181%
15	11.451	1587	1592	1600	rVB3	201821	503791	11.11%	1.021%
16	11.568	1601	1612	1620	rBV3	359343	1504688	33.17%	3.048%
17	11.774	1635	1647	1649	rBV2	751196	2113246	46.58%	4.281%
18	12.286	1731	1734	1735	rBV	316100	331683	7.31%	0.672%
19	12.310	1736	1738	1742	rVV	453603	610737	13.46%	1.237%
20	12.351	1742	1745	1747	rVV	324282	390684	8.61%	0.791%
21	12.921	1837	1842	1845	rBV	4670174	4536369	100.00%	9.190%
22	13.139	1874	1879	1882	rBV4	41991	56825	1.25%	0.115%
23	13.392	1918	1922	1926	rVB	66096	77660	1.71%	0.157%
24	13.480	1933	1937	1940	rBV2	63735	74437	1.64%	0.151%
25	13.804	1989	1992	2000	rBV	499391	701444	15.46%	1.421%
26	13.980	2018	2022	2030	rBV	1504648	1366443	30.12%	2.768%
27	14.127	2044	2047	2051	rVB	143371	130376	2.87%	0.264%
28	14.433	2095	2099	2105	rBV	293270	345676	7.62%	0.700%
29	14.574	2118	2123	2128	rBV5	84278	224834	4.96%	0.455%
30	14.733	2145	2150	2154	rBV	505714	563850	12.43%	1.142%
31	14.809	2160	2163	2165	rBV	54909	62820	1.38%	0.127%
32	15.062	2202	2206	2210	rBV	618251	718650	15.84%	1.456%
33	15.445	2265	2271	2279	rBV2	1180067	1962041	43.25%	3.975%
34	15.803	2324	2332	2333	rBV	391683	758432	16.72%	1.536%

LSC Area Percent Report

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Data File : BF114575.D
Acq On : 24 May 2019 17:52
Operator : JU/SJ
Sample : K2993-16
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

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	16.351	2420	2425	2432	rVB	206792	353935	7.80%	0.717%

Sum of corrected areas: 49363355

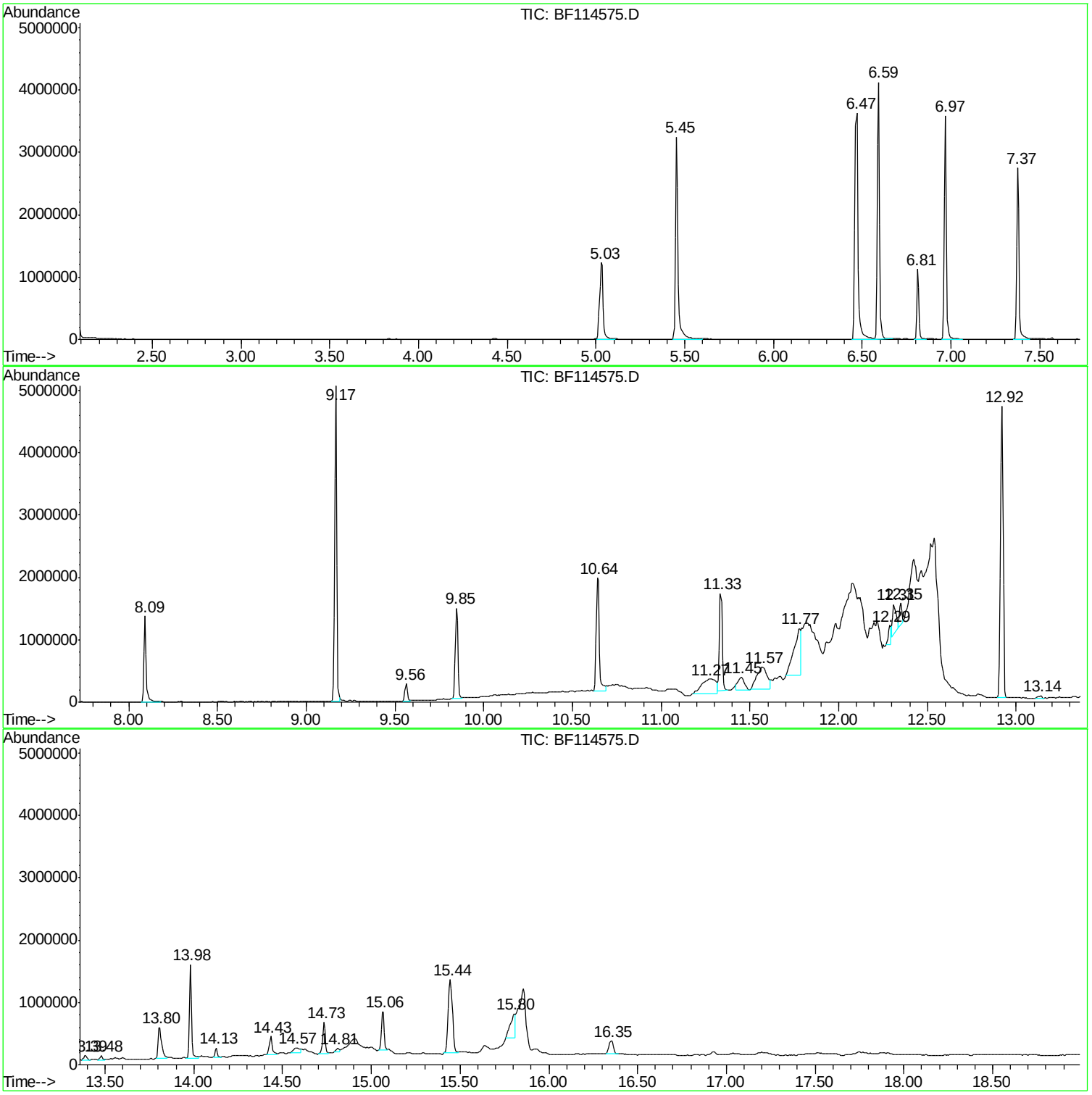
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052419\
Data File : BF114575.D
Acq On : 24 May 2019 17:52
Operator : JU/SJ
Sample : K2993-16
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052419\
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Acq On : 24 May 2019 17:52
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ALS Vial : 4 Sample Multiplier: 1

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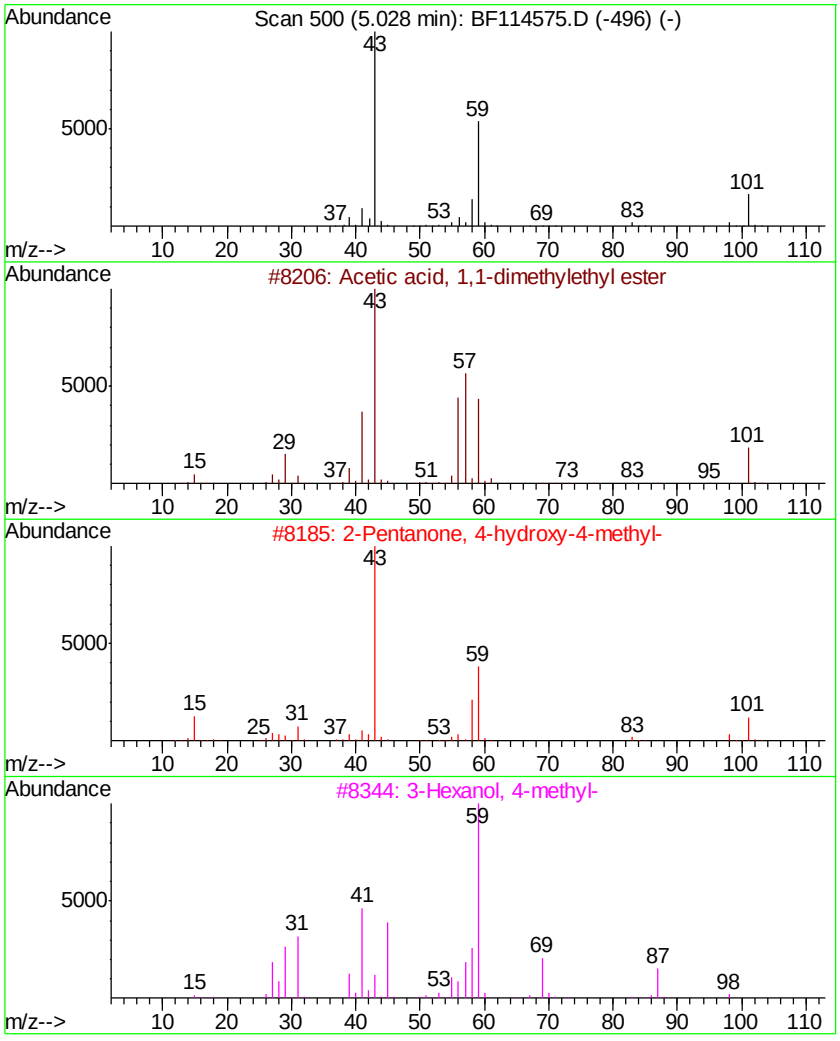
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

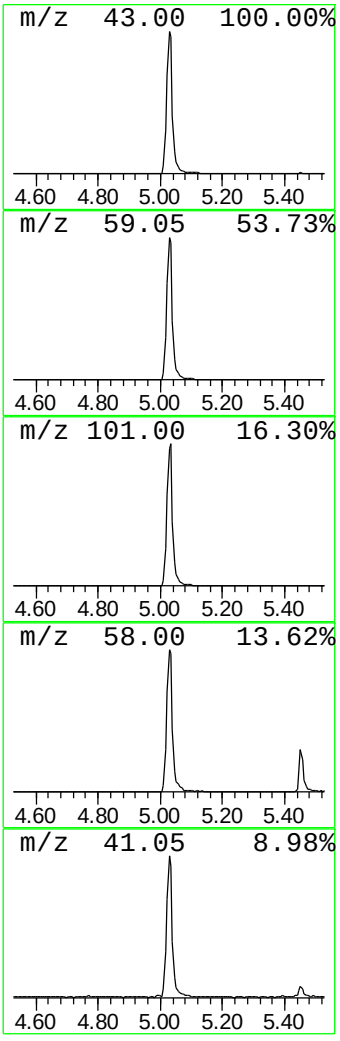
****

Peak Number 1 unknown5.03 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	33.51 ng	1612520	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





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Operator : JU/SJ
Sample : K2993-16
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

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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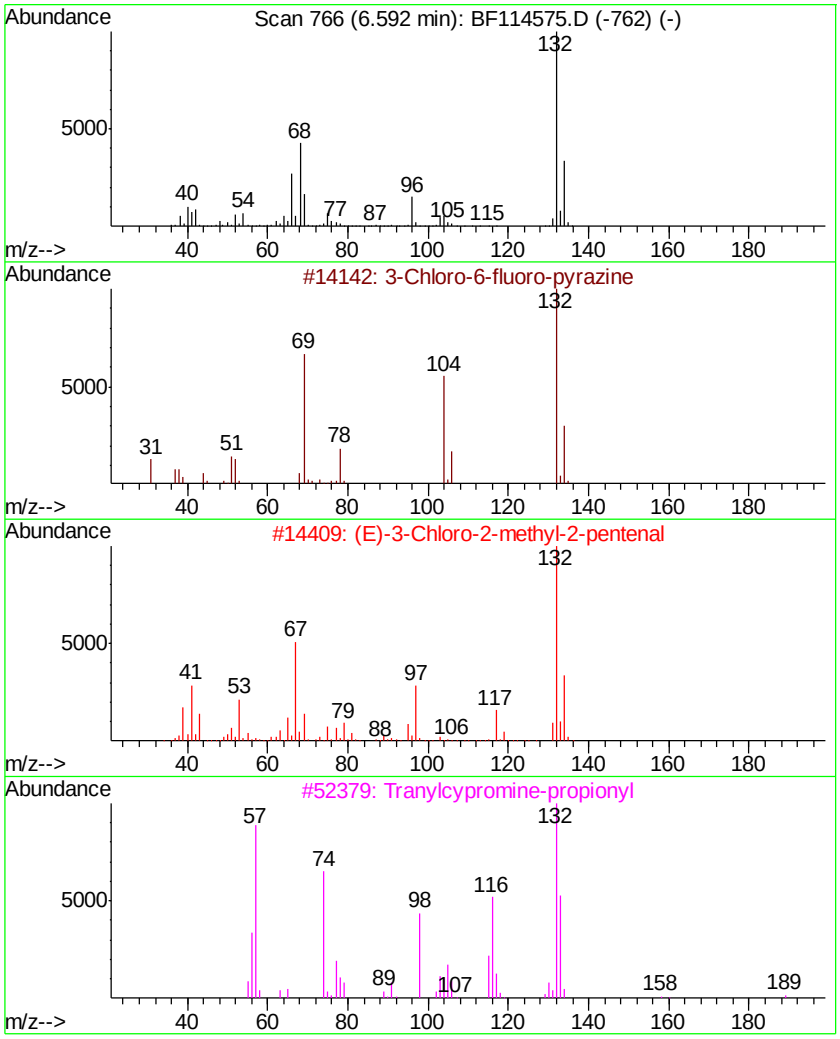
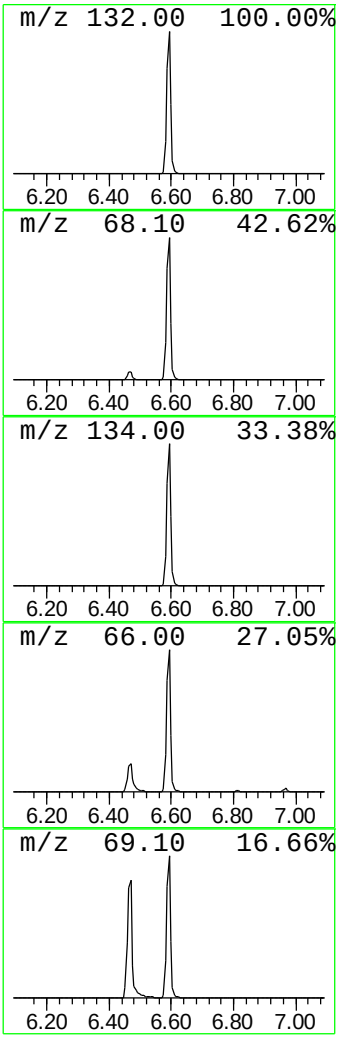
Peak Number 2 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	78.08 ng	3757560	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Data File : BF114575.D
Acq On : 24 May 2019 17:52
Operator : JU/SJ
Sample : K2993-16
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

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

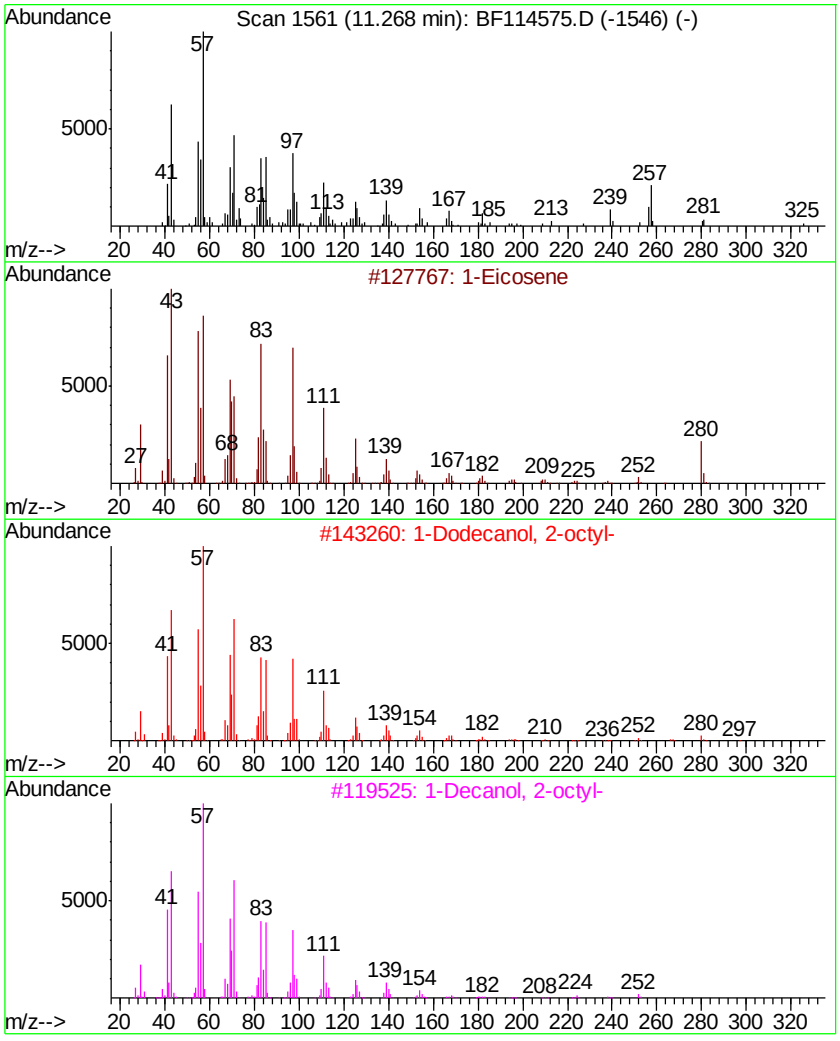
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

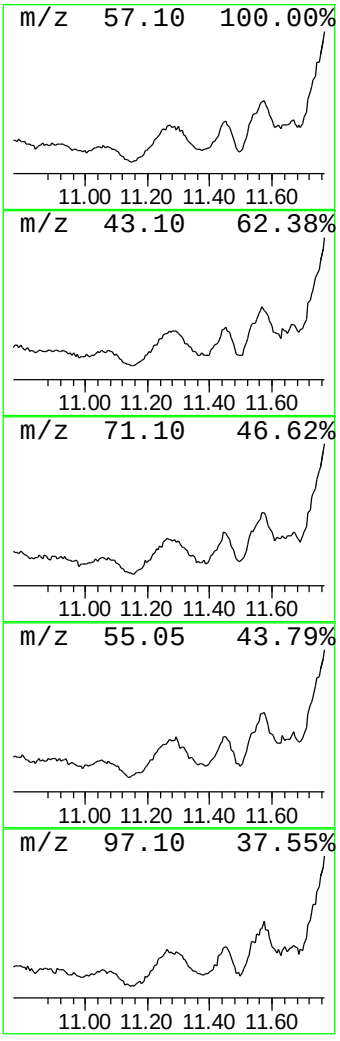
****

Peak Number 4 1-Eicosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.27	16.90 ng	1327040	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosene	280	C20H40	003452-07-1	70
2	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	70
3	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	70
4	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	64
5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	62





Library Search Compound Report

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Data File : BF114575.D
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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

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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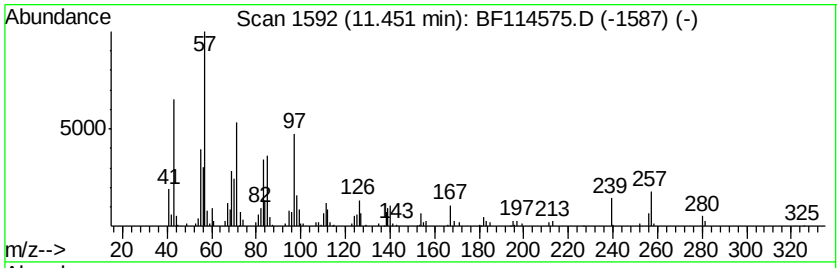
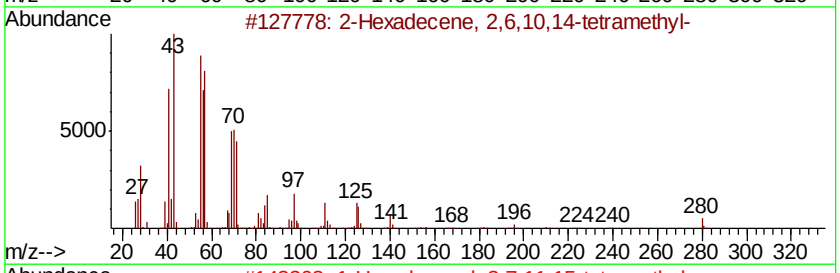
****

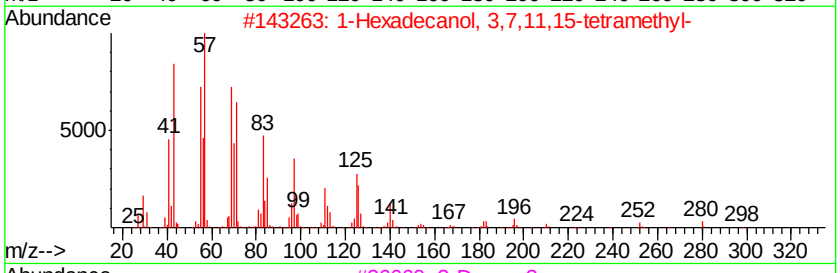
Peak Number 5 2-Hexadecene, 2,6,10,14-tet... Concentration Rank 11

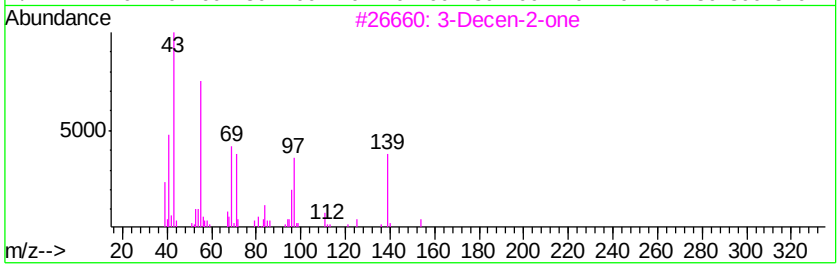
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.45	6.42 ng	503791	Phenanthrene-d10	11.33

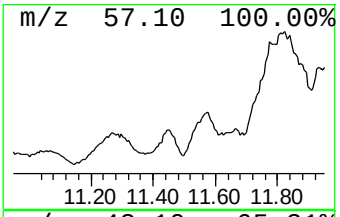
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexadecene, 2,6,10,14-tetramet...	280	C20H40	056554-34-8	50
2	1-Hexadecanol, 3,7,11,15-tetrame...	298	C20H42O	000645-72-7	46
3	3-Decen-2-one	154	C10H18O	010519-33-2	43
4	2-Hexyldecyl propionate	298	C19H38O2	1072781-99-7	38
5	Undecane, 3,4-dimethyl-	184	C13H28	017312-78-6	35

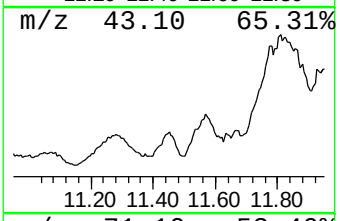


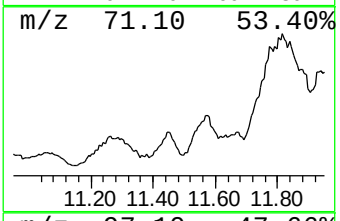


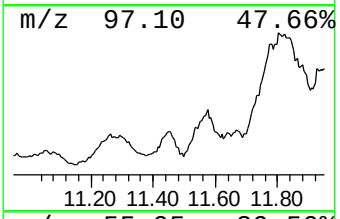


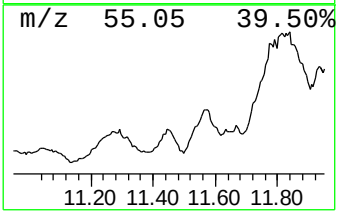












Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : COMP-1

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

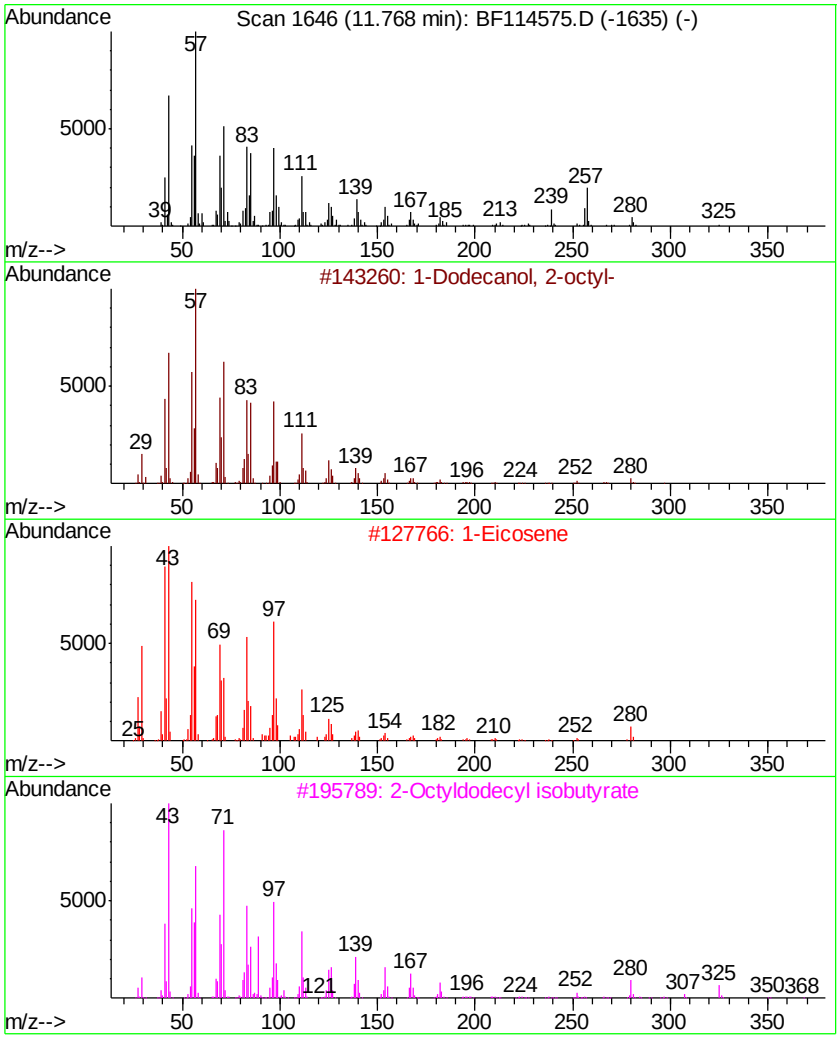
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

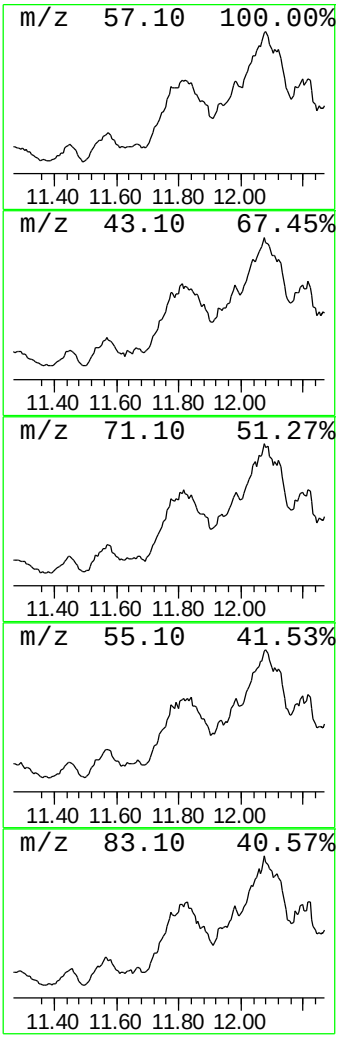
****

Peak Number 7 1-Dodecanol, 2-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	26.92 ng	2113250	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	90
2	1-Eicosene	280	C20H40	003452-07-1	89
3	2-Octyldodecyl isobutyrate	368	C24H48O2	1000368-55-5	83
4	2-Octyldodecyl propionate	354	C23H46O2	1000368-55-1	76
5	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	74





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

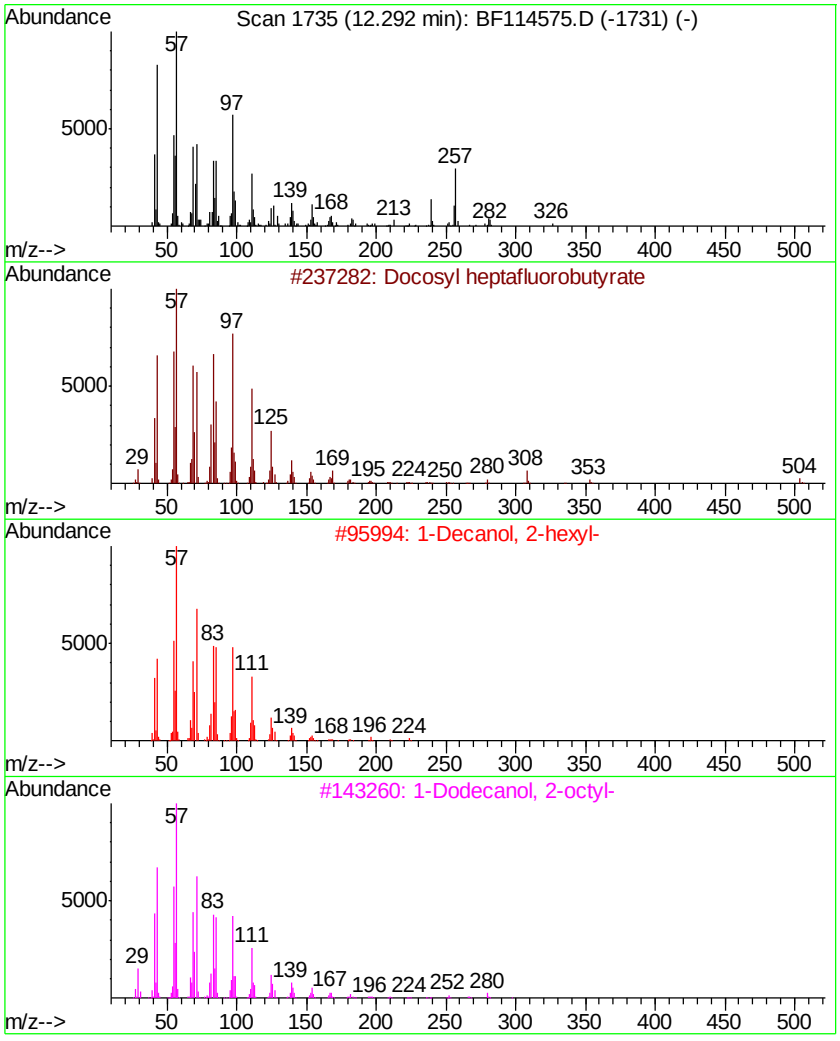
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

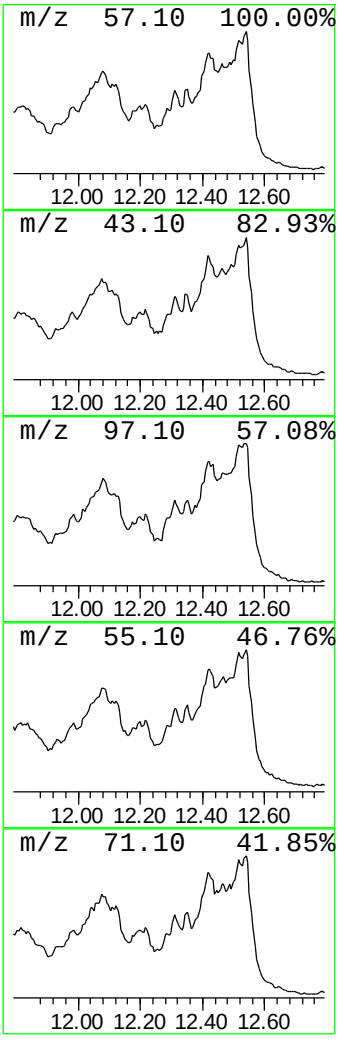
****

Peak Number 8 Docosyl heptafluorobutyrate Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	4.22 ng	331683	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosyl heptafluorobutyrate	522	C26H45F7O2	1000351-83-1	52
2	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	49
3	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	49
4	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	46
5	1-Dodecanol, 2-octyl-, acetate	340	C22H44O2	074051-84-6	46





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

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

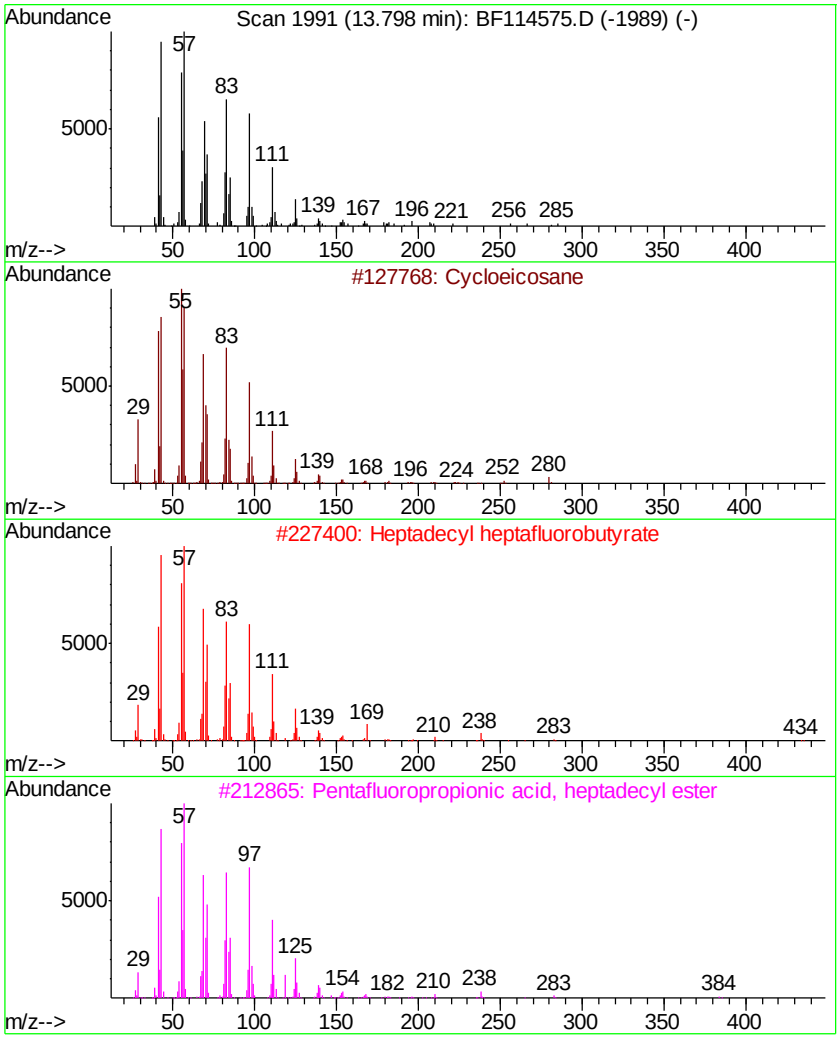
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

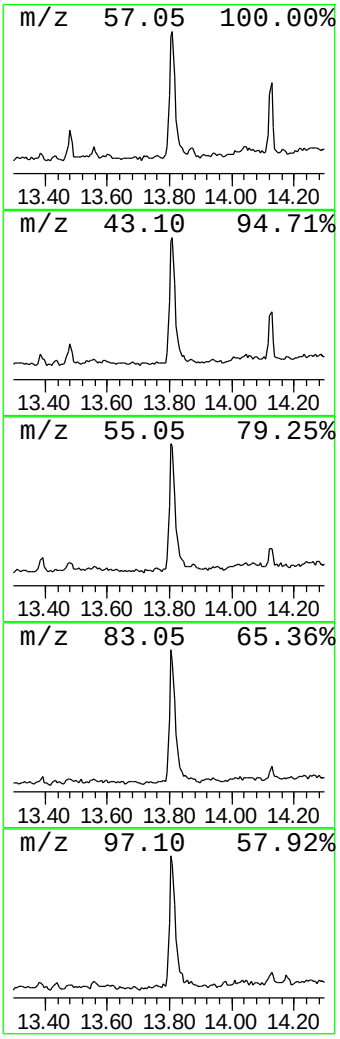
****

Peak Number 11 Cycloeicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	10.27 ng	701444	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	96
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

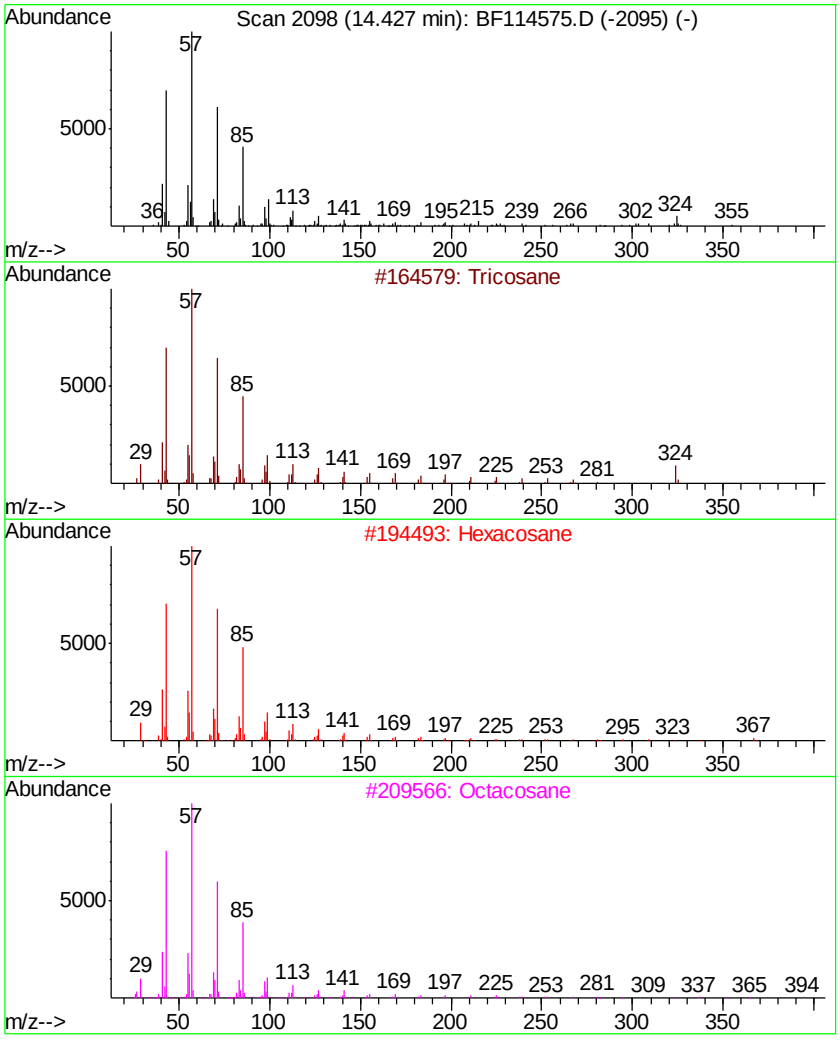
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

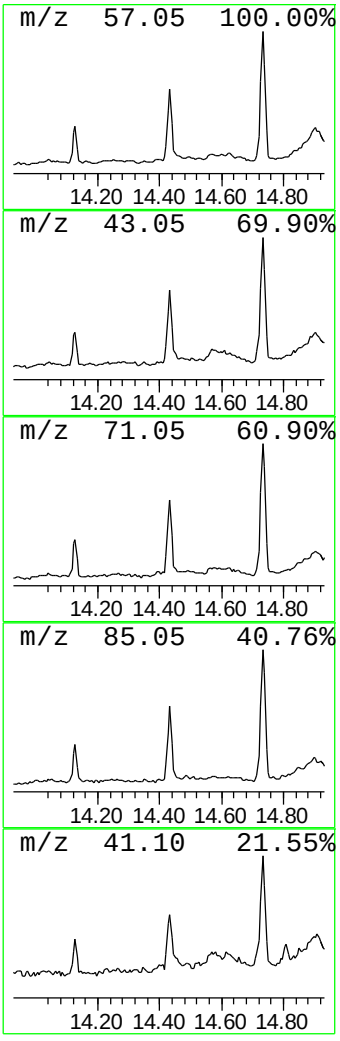
****

Peak Number 12 Tricosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	5.06 ng	345676	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	94
2	Hexacosane	366	C26H54	000630-01-3	91
3	Octacosane	394	C28H58	000630-02-4	90
4	Hexadecane	226	C16H34	000544-76-3	90
5	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052419\
Data File : BF114575.D
Acq On : 24 May 2019 17:52
Operator : JU/SJ
Sample : K2993-16
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

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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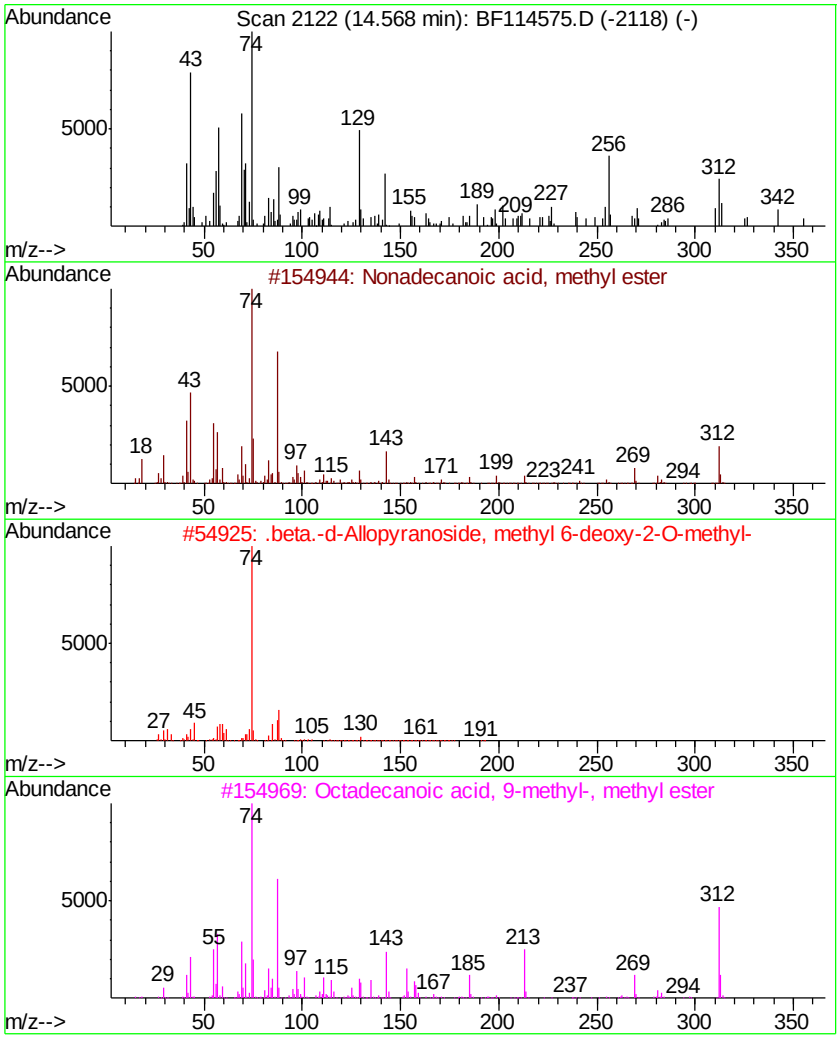
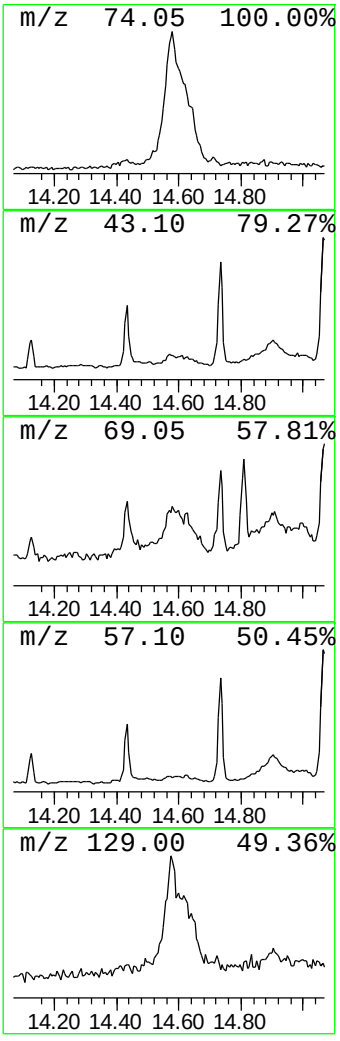
Peak Number 13 unknown14.57 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	3.29 ng	224834	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	25
2	.beta.-d-Allopyranoside, methyl ...	192	C8H16O5	014917-72-7	16
3	Octadecanoic acid, 9-methyl-, me...	312	C20H40O2	014066-50-3	16
4	Propanamide, N-cyclohexyl-	155	C9H17NO	001126-56-3	14
5	Methyl valerate	116	C6H12O2	000624-24-8	14





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Data File : BF114575.D
Acq On : 24 May 2019 17:52
Operator : JU/SJ
Sample : K2993-16
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

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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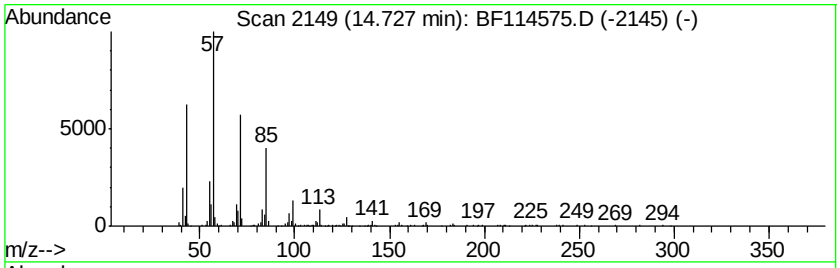
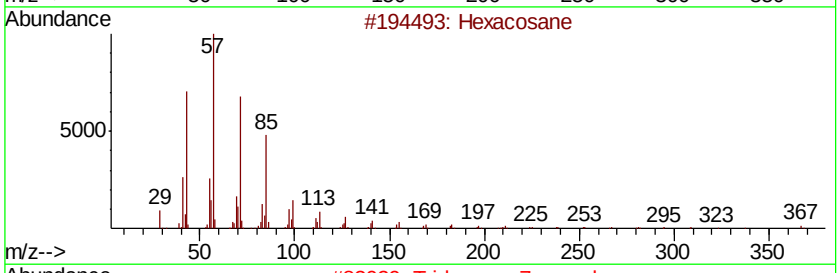
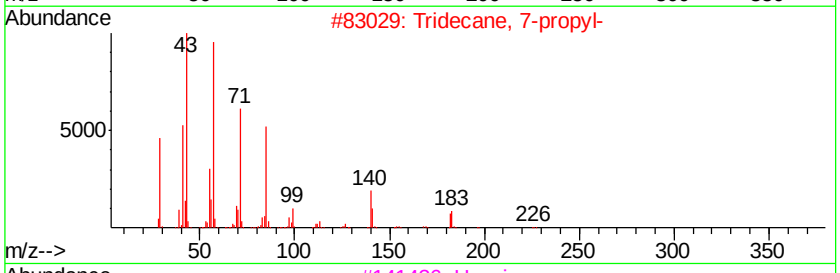
Peak Number 14 Hexacosane Concentration Rank 12

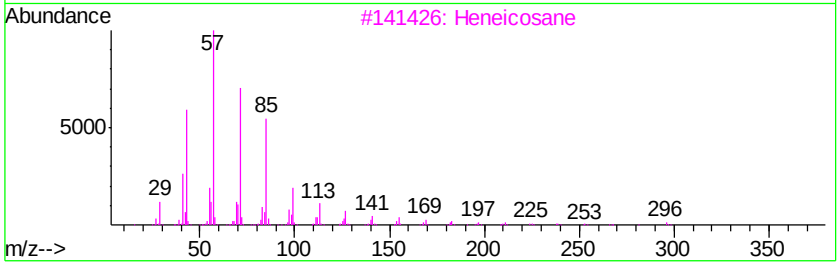
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	5.75 ng	563850	Perylene-d12	15.45

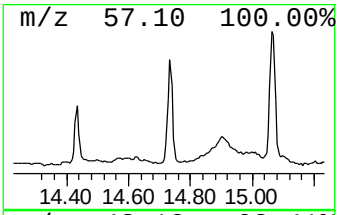
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Tridecane, 7-propyl-	226	C16H34	055045-09-5	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Pentacosane	352	C25H52	000629-99-2	90
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87

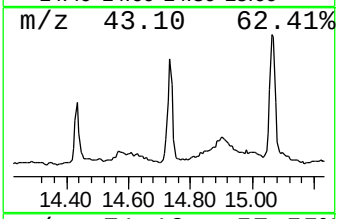


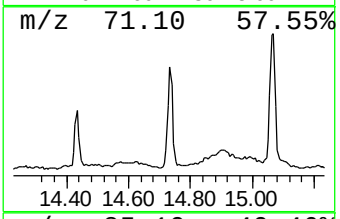


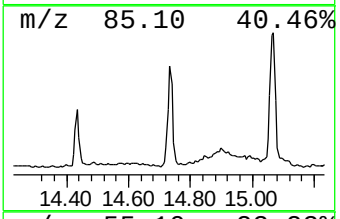


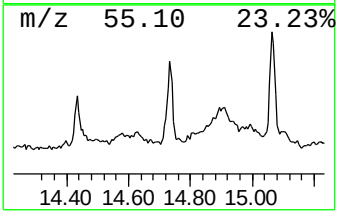












Library Search Compound Report

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Data File : BF114575.D
Acq On : 24 May 2019 17:52
Operator : JU/SJ
Sample : K2993-16
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

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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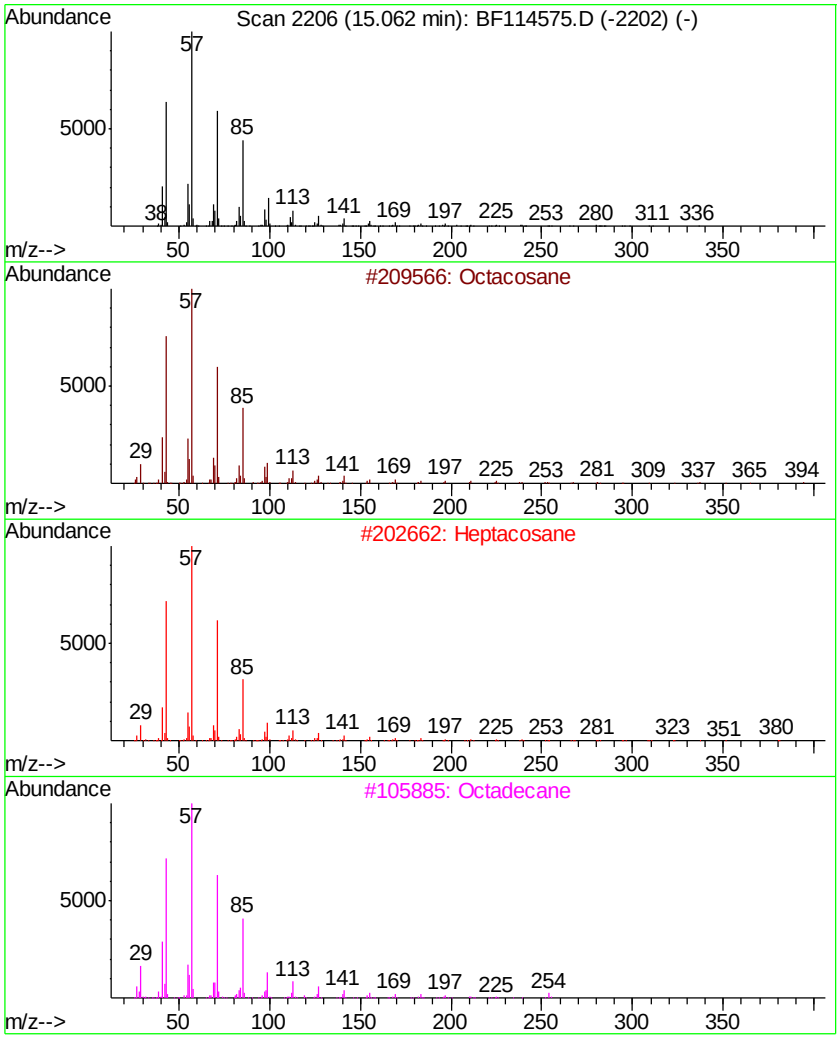
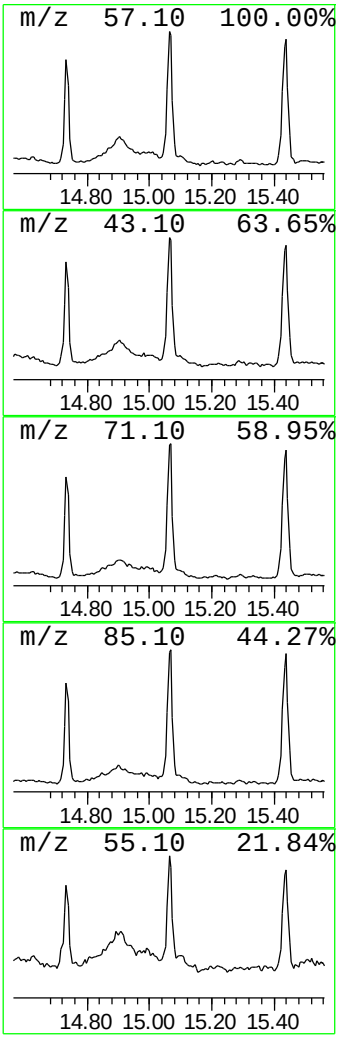
Peak Number 15 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	7.33 ng	718650	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Octadecane	254	C18H38	000593-45-3	86
4	Pentacosane	352	C25H52	000629-99-2	86
5	Tridecane, 6-propyl-	226	C16H34	055045-10-8	83





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Data File : BF114575.D
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Sample : K2993-16
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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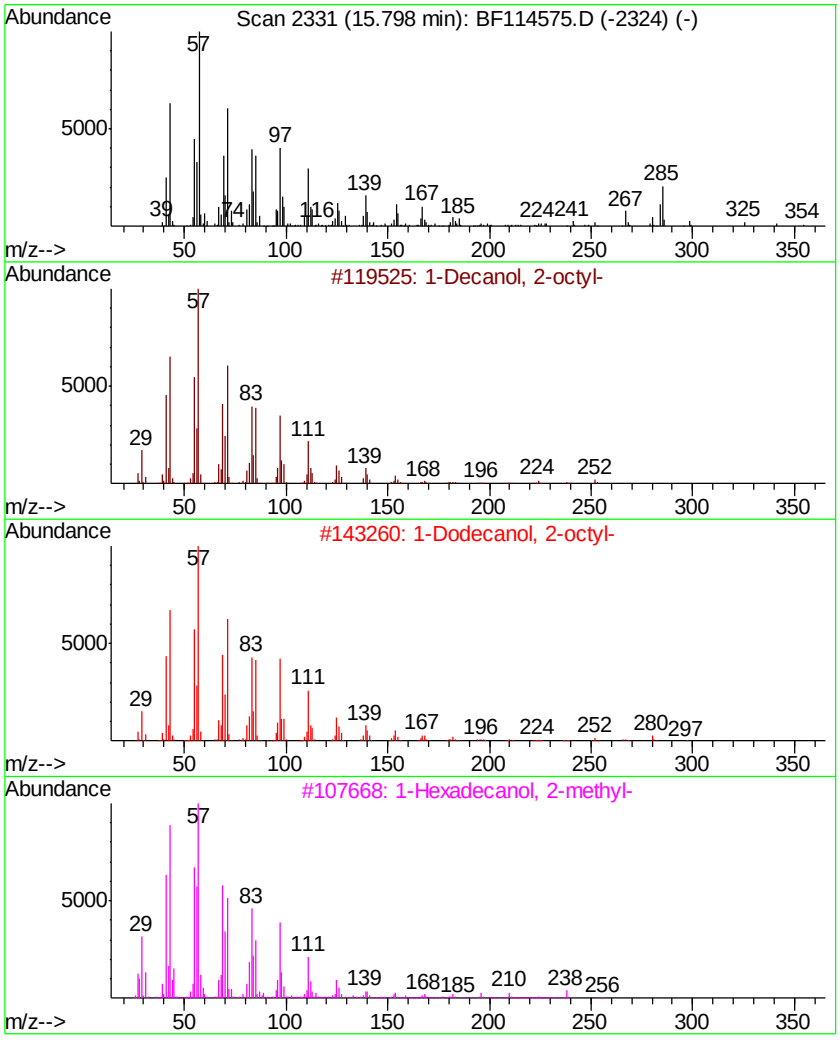
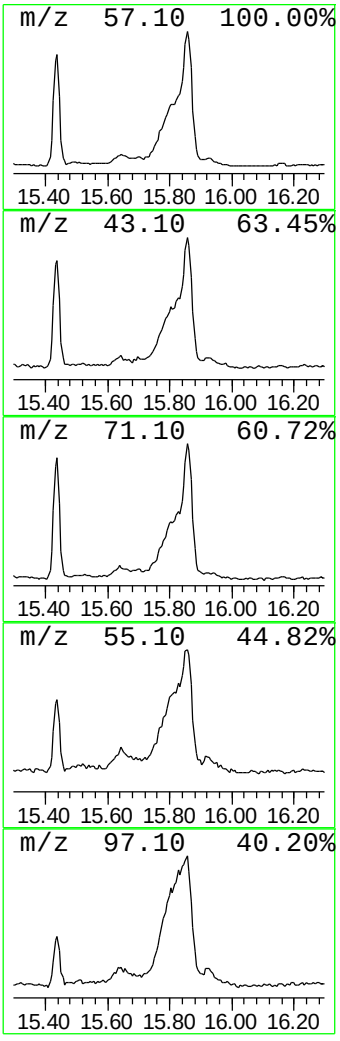
Peak Number 16 1-Decanol, 2-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	7.73 ng	758432	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	81
2	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	81
3	1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	78
4	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	76
5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF052419\
Data File : BF114575.D
Acq On : 24 May 2019 17:52
Operator : JU/SJ
Sample : K2993-16
Misc :
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Instrument : BNA_F
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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
unknown5.03	5.03	33.5	ng	1612520	1	6.81	962434	20.0
unknown6.59	6.59	78.1	ng	3757560	1	6.81	962434	20.0
1-Eicosene	11.27	16.9	ng	1327040	4	11.33	1570110	20.0
2-Hexadecene, 2,6...	11.45	6.4	ng	503791	4	11.33	1570110	20.0
1-Dodecanol, 2-oc...	11.77	26.9	ng	2113250	4	11.33	1570110	20.0
Docosyl heptafluo...	12.29	4.2	ng	331683	4	11.33	1570110	20.0
Cycloeicosane	13.80	10.3	ng	701444	5	13.98	1366440	20.0
Tricosane	14.43	5.1	ng	345676	5	13.98	1366440	20.0
unknown14.57	14.57	3.3	ng	224834	5	13.98	1366440	20.0
Hexacosane	14.73	5.8	ng	563850	6	15.45	1962040	20.0
Octacosane	15.06	7.3	ng	718650	6	15.45	1962040	20.0
1-Decanol, 2-octyl-	15.80	7.7	ng	758432	6	15.45	1962040	20.0