LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061720\
Data File : BF120635.D
Acq On : 17 Jun 2020 16:28
Operator : JU/CG
Sample : L3020-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-24(19-21)

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-BF061020.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	5.410	560	565	568	rBV	4076933	4559121	71.06%	9.952%
2	6.434	733	739	742	rBV	3816925	4802116	74.85%	10.482%
3	6.798	797	801	804	rBV	1186657	927009	14.45%	2.023%
4	6.957	823	828	831	rBV	4348143	3946899	61.52%	8.615%
5	7.363	891	897	900	rBV	3291953	3247312	50.62%	7.088%
6	8.075	1015	1018	1022	rBV	1311155	1208089	18.83%	2.637%
7	9.157	1197	1202	1205	rBV	5847339	5678330	88.51%	12.395%
8	9.545	1265	1268	1271	rBV	1139546	839391	13.08%	1.832%
9	9.751	1295	1303	1311	rBV2	39176	82453	1.29%	0.180%
10	9.828	1313	1316	1320	rVB	1604522	1418348	22.11%	3.096%
11	10.622	1446	1451	1454	rBV	3841799	3792093	59.11%	8.277%
12	11.316	1565	1569	1572	rBV	1651786	1529910	23.85%	3.339%
13	11.527	1602	1605	1616	rVB	69793	71382	1.11%	0.156%
14	12.721	1804	1808	1811	rBV	89118	70608	1.10%	0.154%
15	12.780	1814	1818	1830	rBV	200530	238651	3.72%	0.521%
16	12.904	1833	1839	1842	rBV	5776699	6415627	100.00%	14.004%
17	13.451	1930	1932	1935	rBV	72707	67483	1.05%	0.147%
18	13.798	1987	1991	2004	rBV	301982	513726	8.01%	1.121%
19	13.945	2012	2016	2020	rBV	1618317	1565386	24.40%	3.417%
20	14.115	2042	2045	2051	rBV	148878	130480	2.03%	0.285%
21	14.421	2093	2097	2100	rBV	261139	220211	3.43%	0.481%
22	14.704	2141	2145	2152	rBV2	1199482	1545614	24.09%	3.374%
23	15.045	2199	2203	2209	rBV	311840	354299	5.52%	0.773%
24	15.386	2255	2261	2264	rBV	1385505	1698659	26.48%	3.708%
25	15.415	2264	2266	2273	rVB	293441	316329	4.93%	0.690%
26	15.833	2332	2337	2343	rBV	198781	287398	4.48%	0.627%
27	16.321	2415	2420	2435	rVB	109761	209399	3.26%	0.457%
28	16.892	2513	2517	2526	rVB2	38526	76426	1.19%	0.167%

Sum of corrected areas: 45812749

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061720\
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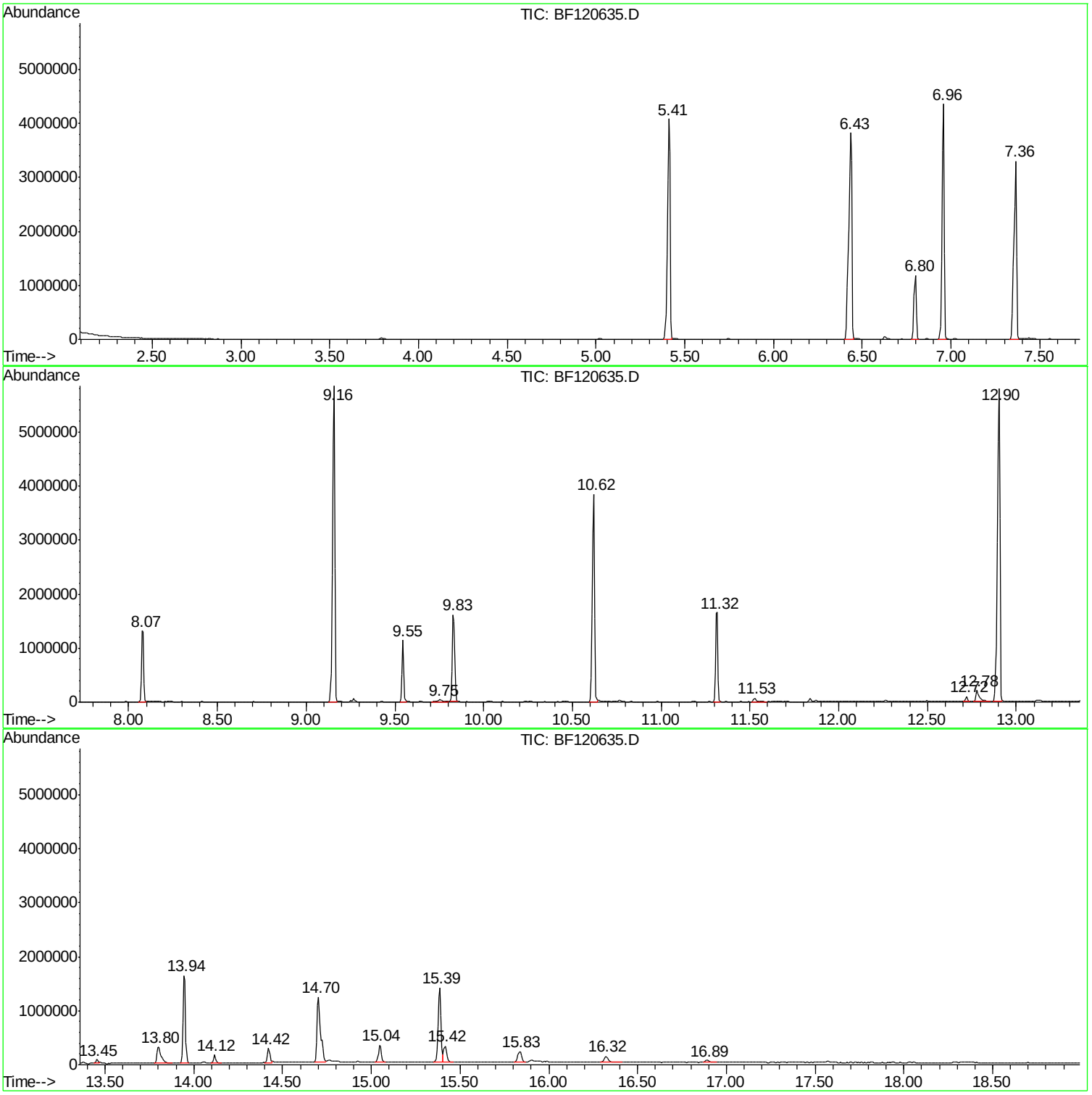
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-24(19-21)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061020.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\BF061720\
Data File : BF120635.D
Acq On : 17 Jun 2020 16:28
Operator : JU/CG
Sample : L3020-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-24(19-21)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061020.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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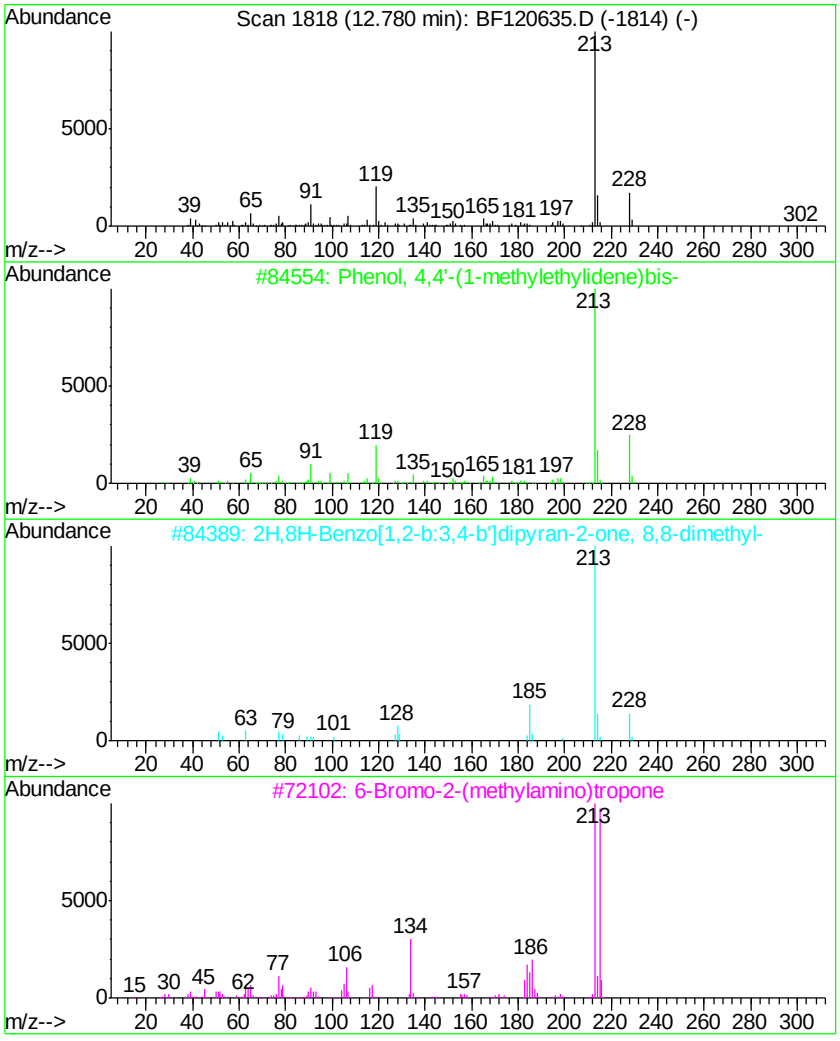
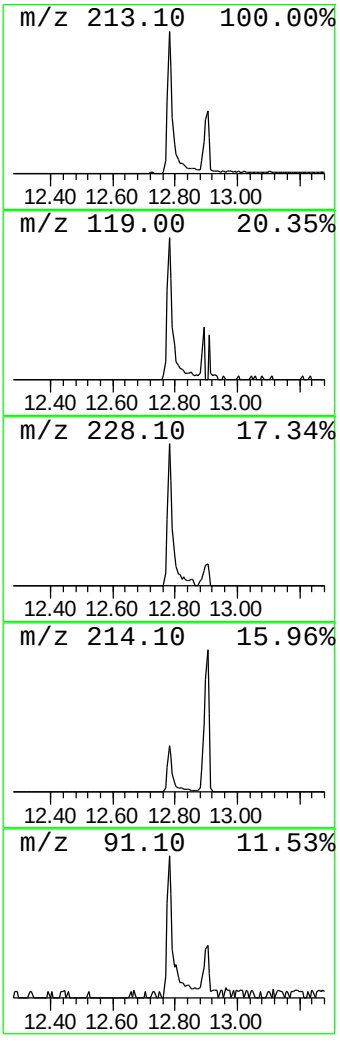
Peak Number 2 Phenol, 4,4'-(1-methylethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	3.05 ng	238651	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	98
2	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	53
3	6-Bromo-2-(methylamino)tropone	213	C8H8BrNO	1000241-43-1	50
4	2,5-bis(Trimethylsilyl)thiophene	228	C10H20SSi2	017906-71-7	42
5	Acridine, 9-chloro-	213	C13H8ClN	001207-69-8	40





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061720\
Data File : BF120635.D
Acq On : 17 Jun 2020 16:28
Operator : JU/CG
Sample : L3020-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-24(19-21)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061020.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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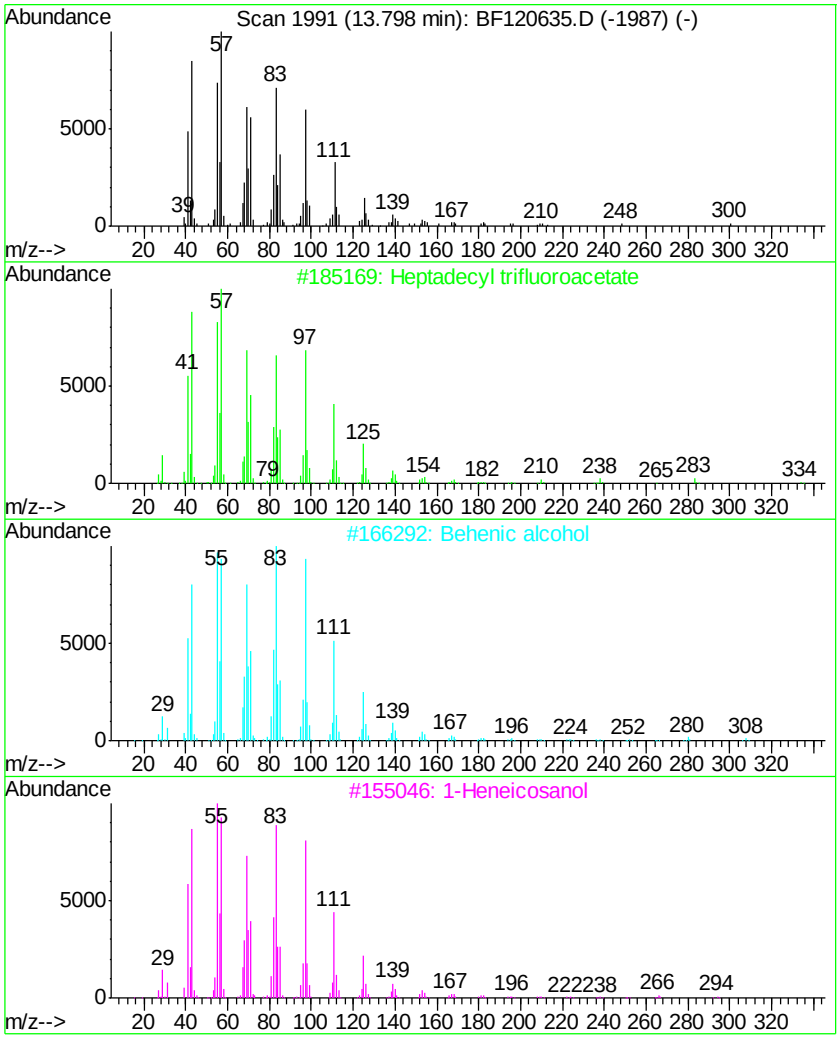
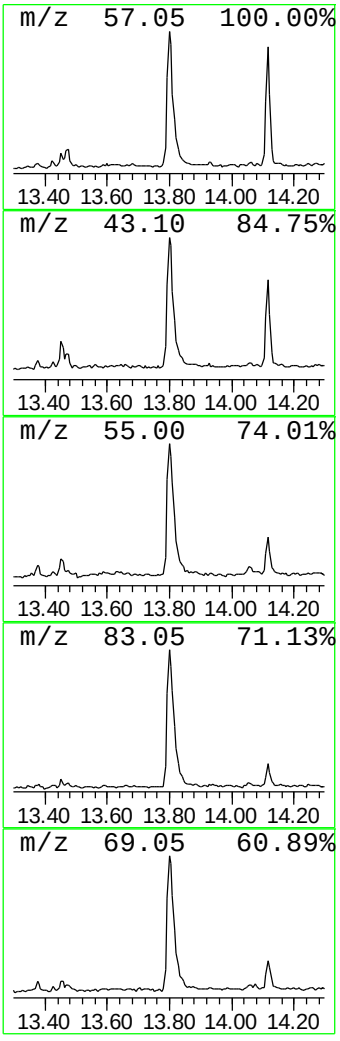
Peak Number 3 Heptadecyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	6.56 ng	513726	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061720\
Data File : BF120635.D
Acq On : 17 Jun 2020 16:28
Operator : JU/CG
Sample : L3020-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-24(19-21)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061020.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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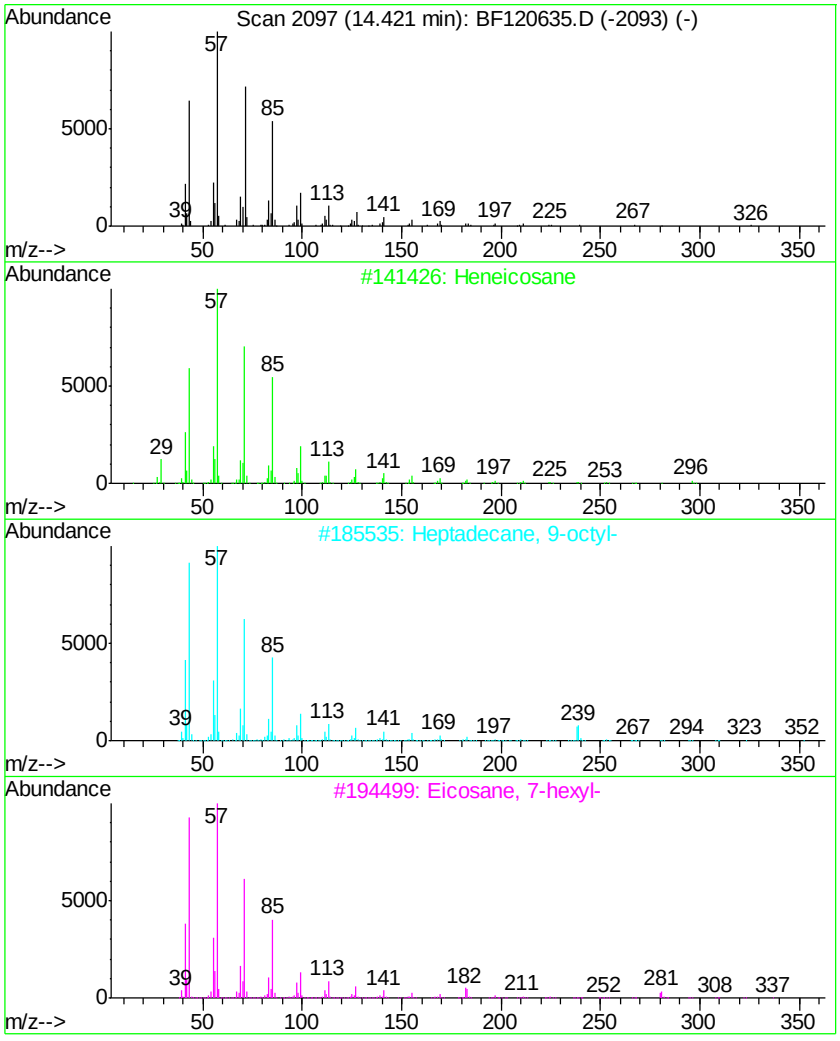
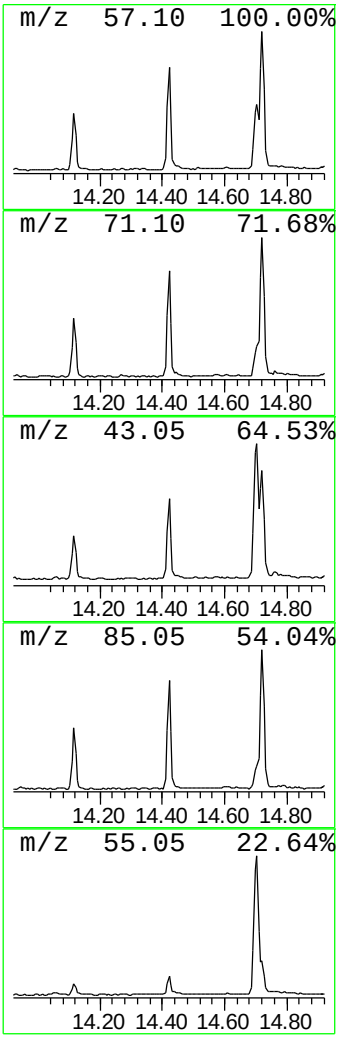
Peak Number 4 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.42	2.81 ng	220211	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Heptadecane	240	C17H36	000629-78-7	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061720\
Data File : BF120635.D
Acq On : 17 Jun 2020 16:28
Operator : JU/CG
Sample : L3020-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-24(19-21)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061020.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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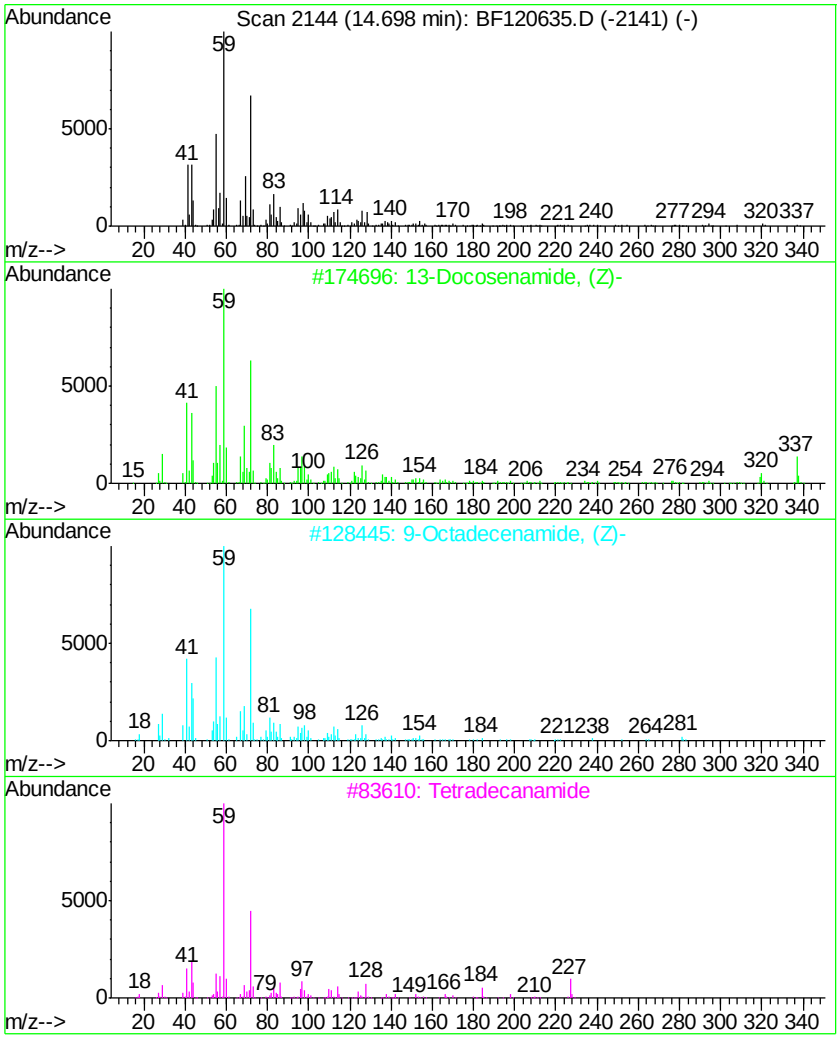
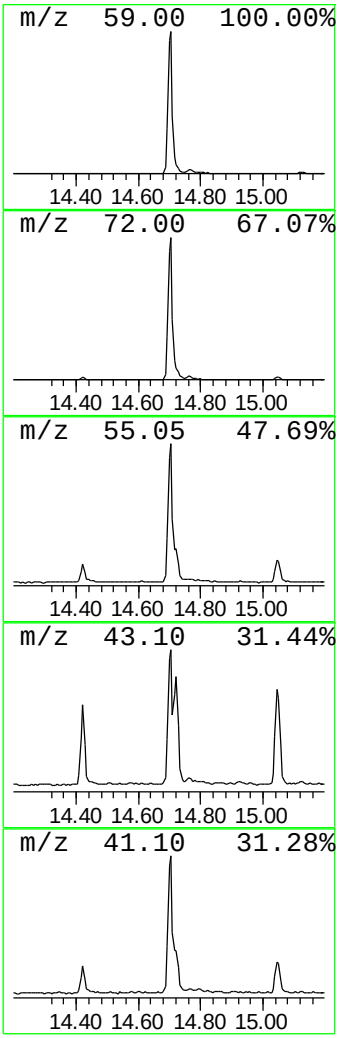
Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	18.20 ng	1545610	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	94
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3	Tetradecanamide	227	C14H29NO	000638-58-4	64
4	Octadecanamide	283	C18H37NO	000124-26-5	47
5	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061720\
Data File : BF120635.D
Acq On : 17 Jun 2020 16:28
Operator : JU/CG
Sample : L3020-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-24(19-21)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061020.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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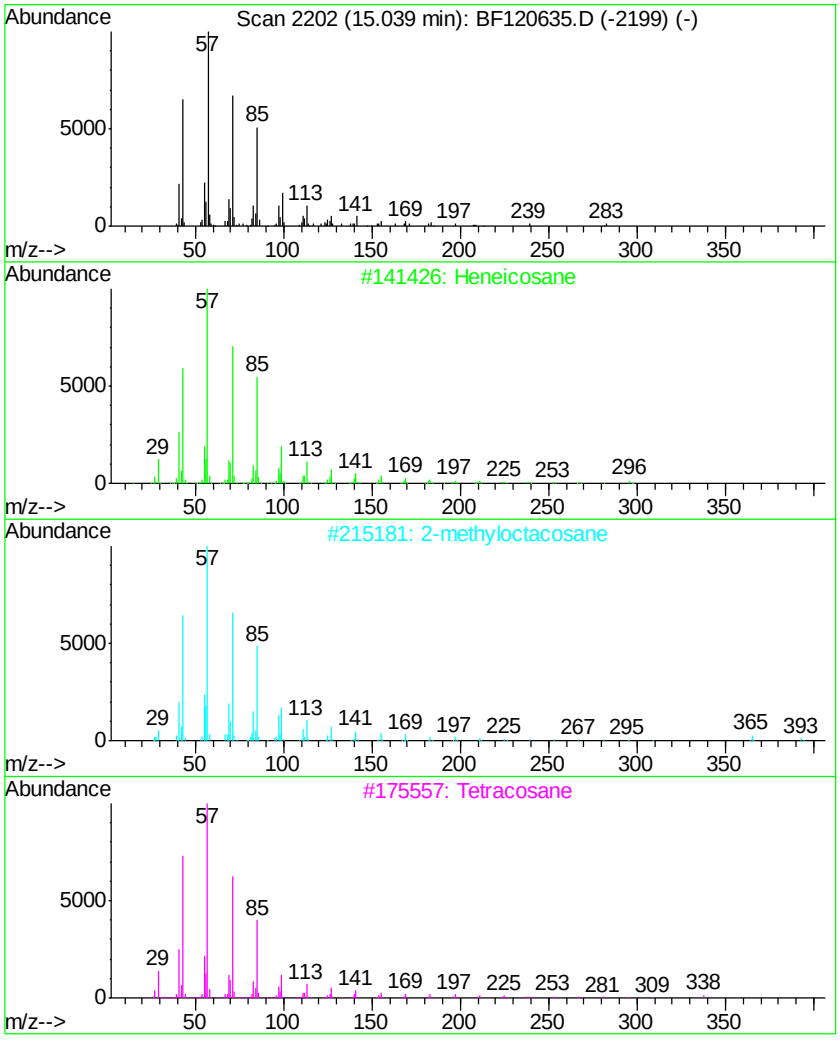
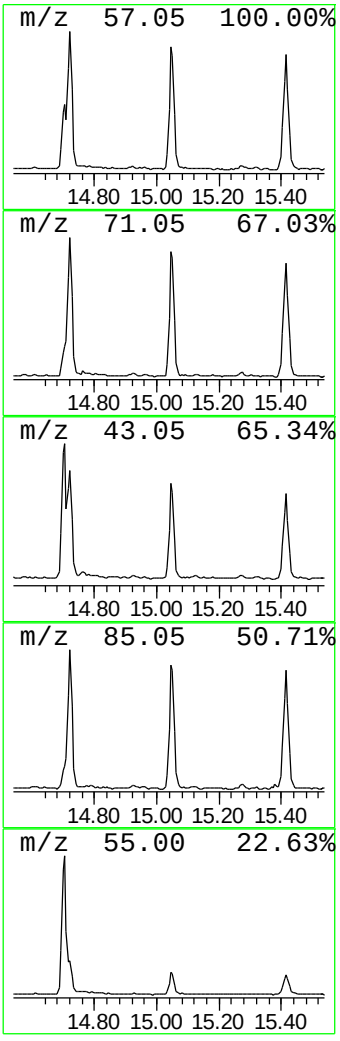
Peak Number 6 2-methyloctacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	4.17 ng	354299	Perylene-d12	15.39

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	Tetracosane	338	C24H50	000646-31-1	91
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061720\
Data File : BF120635.D
Acq On : 17 Jun 2020 16:28
Operator : JU/CG
Sample : L3020-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-24(19-21)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061020.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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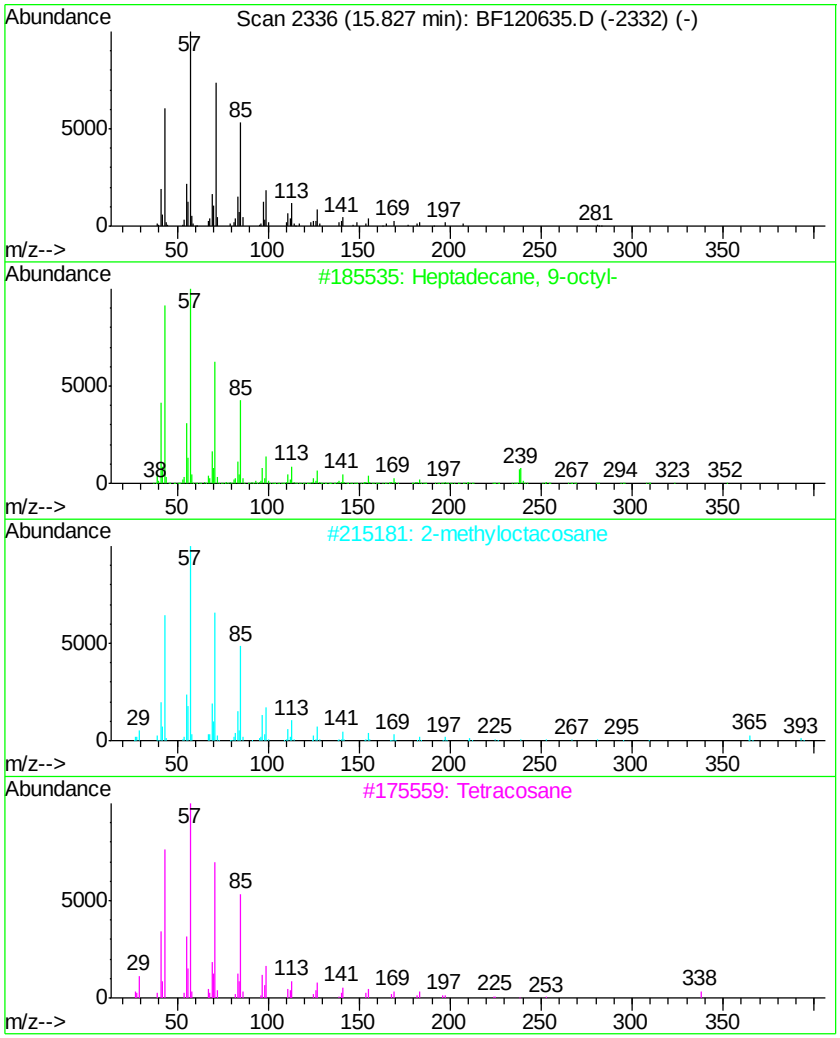
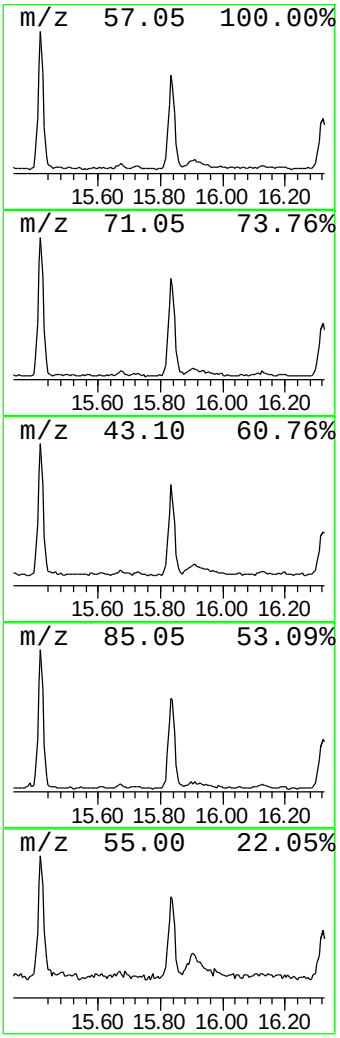
Peak Number 7 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	3.38 ng	287398	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Hexacosane	366	C26H54	000630-01-3	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061720\
Data File : BF120635.D
Acq On : 17 Jun 2020 16:28
Operator : JU/CG
Sample : L3020-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-24(19-21)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061020.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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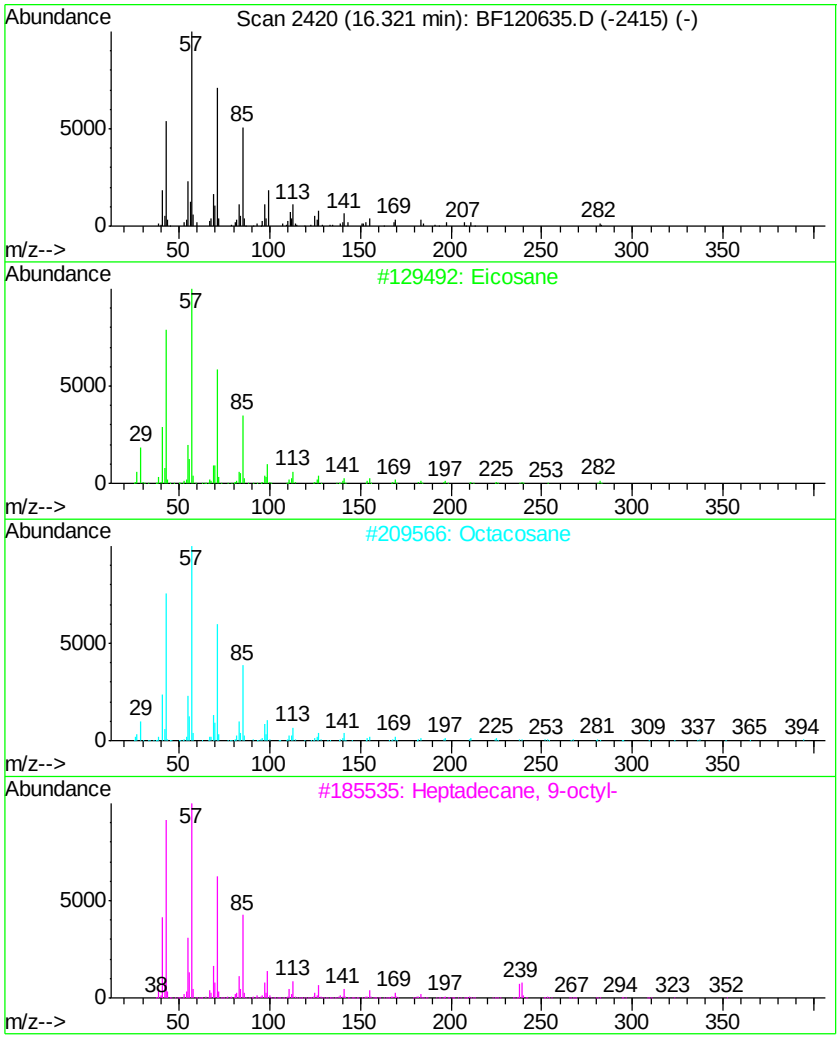
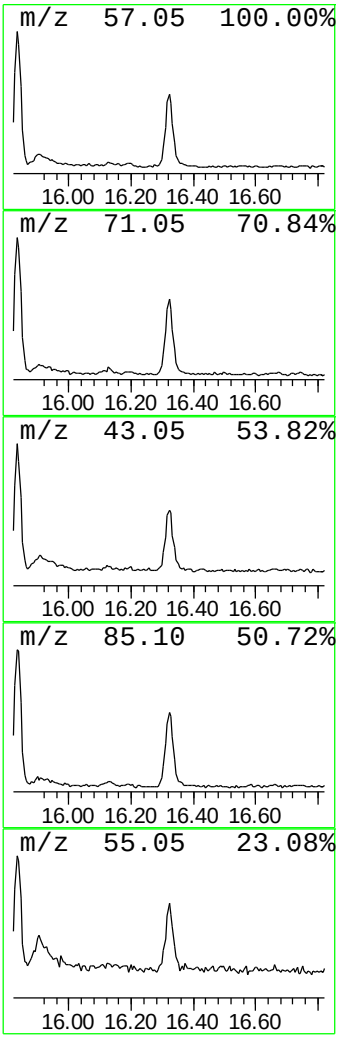
Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	2.47 ng	209399	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Octacosane	394	C28H58	000630-02-4	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	Heneicosane	296	C21H44	000629-94-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061720\
Data File : BF120635.D
Acq On : 17 Jun 2020 16:28
Operator : JU/CG
Sample : L3020-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-24(19-21)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061020.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
Phenol, 4,4'-(1-m...	12.78	3.0	ng	238651	5	13.94	1565390	20.0
Heptadecyl triflu...	13.80	6.6	ng	513726	5	13.94	1565390	20.0
Heneicosane	14.42	2.8	ng	220211	5	13.94	1565390	20.0
13-Docosenamide, ...	14.70	18.2	ng	1545610	6	15.39	1698660	20.0
2-methyloctacosane	15.04	4.2	ng	354299	6	15.39	1698660	20.0
Heptadecane, 9-oc...	15.83	3.4	ng	287398	6	15.39	1698660	20.0
Eicosane	16.32	2.5	ng	209399	6	15.39	1698660	20.0