LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
Data File : BF118003.D
Acq On : 26 Nov 2019 13:28
Operator : JU
Sample : PB125092BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB125092BL

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-BF111319.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	2.205	10	20	25	rBV	3866451	5458679	98.67%	11.760%
2	5.110	509	514	521	rVB	391092	506384	9.15%	1.091%
3	5.510	577	582	585	rBV	3186229	2992221	54.09%	6.446%
4	6.516	748	753	756	rBV	2496368	2160863	39.06%	4.655%
5	6.663	773	778	781	rBV	4554820	4336595	78.39%	9.343%
6	6.892	813	817	820	rBV	1124492	948042	17.14%	2.042%
7	7.051	839	844	847	rBV	3776482	3367233	60.87%	7.254%
8	7.457	907	913	916	rBV	2732959	2774592	50.16%	5.978%
9	8.175	1031	1035	1039	rBV	1356034	1262693	22.83%	2.720%
10	9.257	1214	1219	1222	rBV	5170740	5132589	92.78%	11.058%
11	9.939	1331	1335	1339	rBV	1820240	1567364	28.33%	3.377%
12	10.733	1465	1470	1474	rBV	3551196	3550203	64.18%	7.649%
13	11.433	1585	1589	1592	rBV	1988902	1637603	29.60%	3.528%
14	13.027	1855	1860	1863	rBV	5266199	5532015	100.00%	11.918%
15	14.080	2035	2039	2043	rBV	1404898	1331130	24.06%	2.868%
16	14.239	2063	2066	2077	rVB	88925	103437	1.87%	0.223%
17	14.545	2113	2118	2122	rBV	176919	179112	3.24%	0.386%
18	14.863	2167	2172	2178	rVB	287447	310739	5.62%	0.669%
19	15.210	2226	2231	2241	rVB	395422	471715	8.53%	1.016%
20	15.586	2289	2295	2297	rBV	889545	1243515	22.48%	2.679%
21	15.610	2297	2299	2310	rVB	434851	505979	9.15%	1.090%
22	16.062	2370	2376	2384	rBV	325021	498181	9.01%	1.073%
23	16.592	2460	2466	2475	rVB	167923	319365	5.77%	0.688%
24	17.209	2566	2571	2581	rVB3	55627	123357	2.23%	0.266%
25	17.945	2689	2696	2704	rBV5	33697	103030	1.86%	0.222%

Sum of corrected areas: 46416636

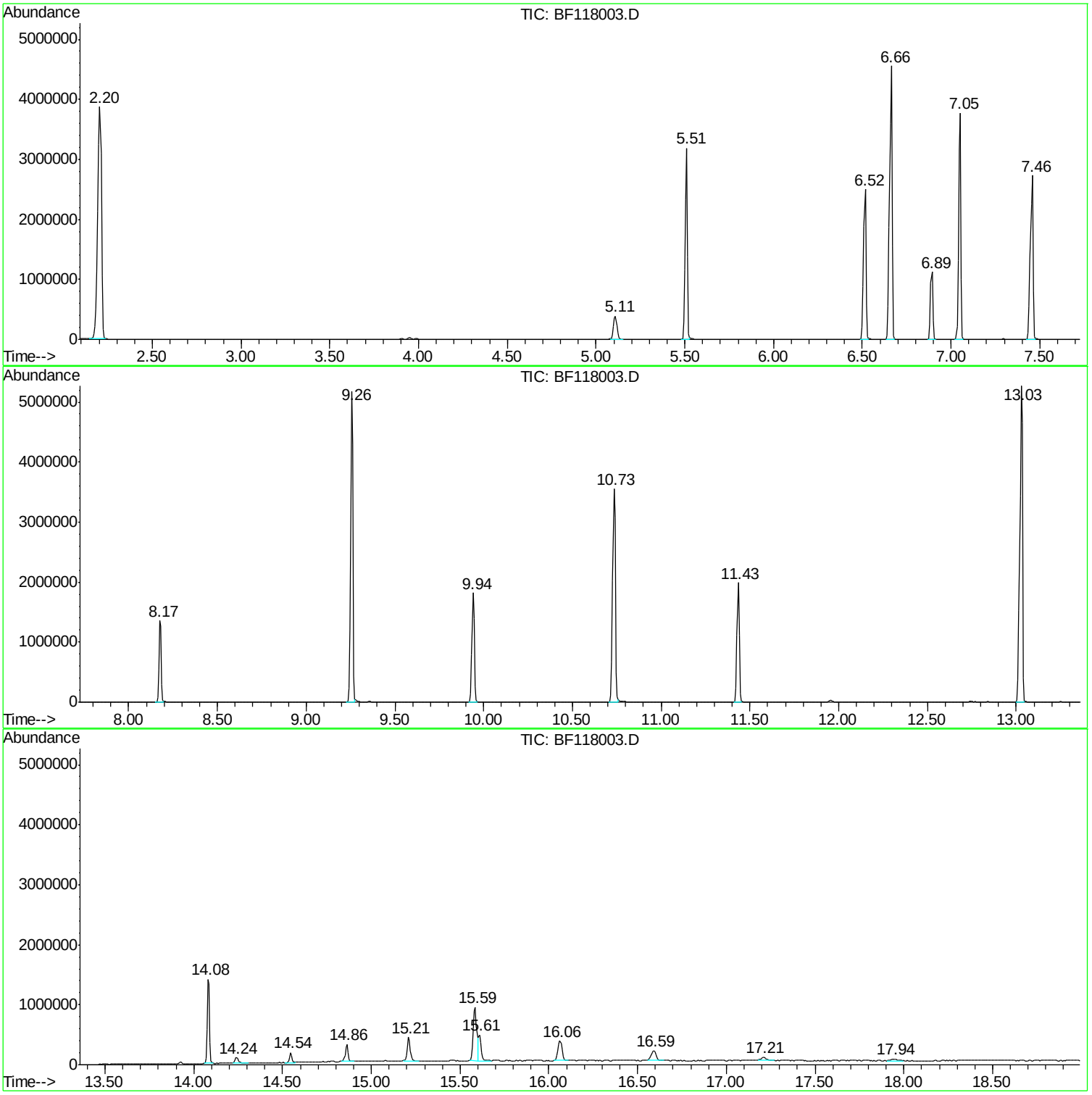
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
Data File : BF118003.D
Acq On : 26 Nov 2019 13:28
Operator : JU
Sample : PB125092BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB125092BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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\BF112619\
Data File : BF118003.D
Acq On : 26 Nov 2019 13:28
Operator : JU
Sample : PB125092BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB125092BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

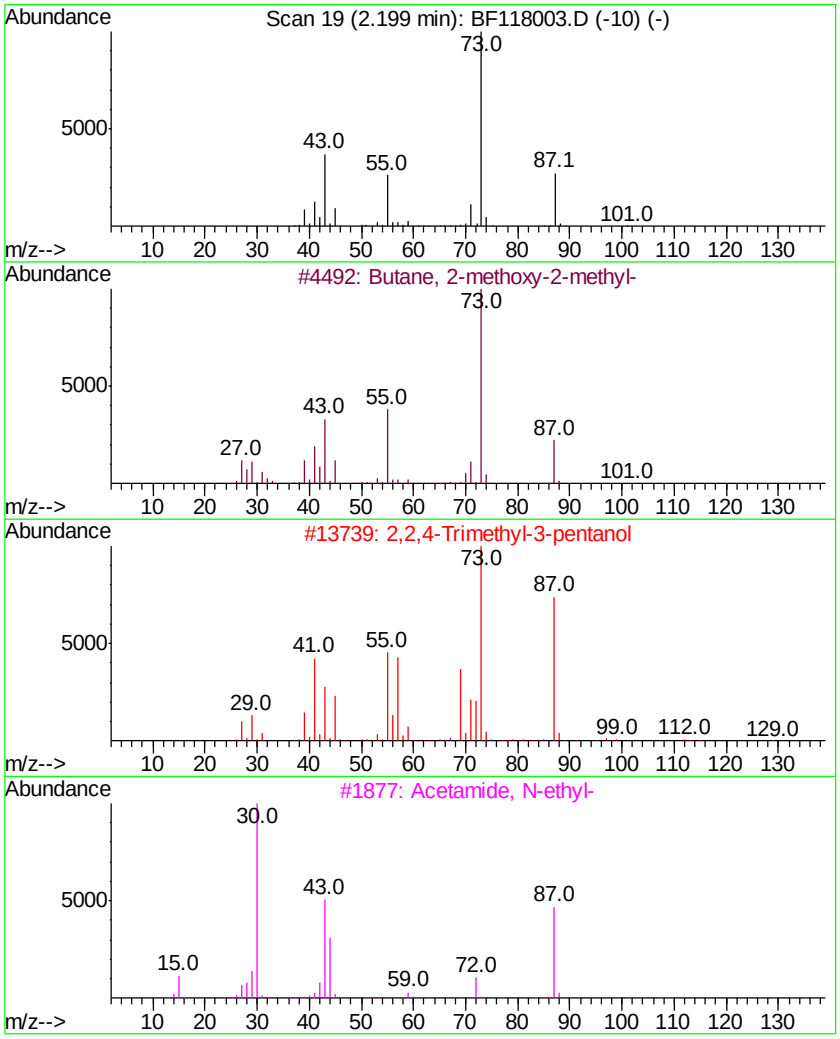
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

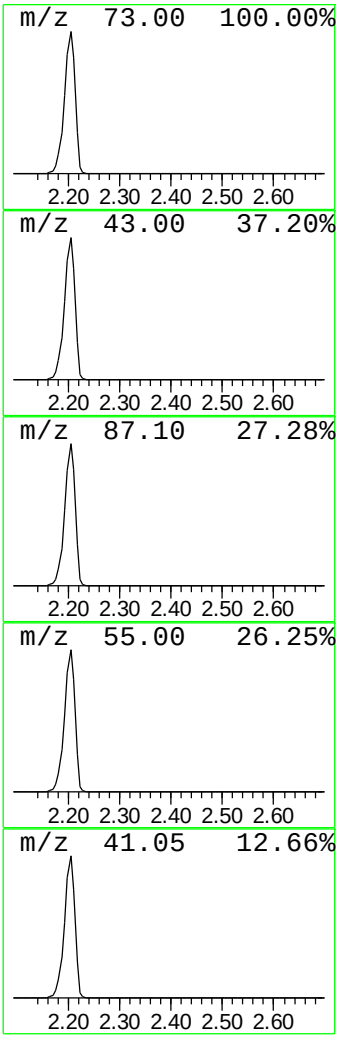
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	115.16 ng	5458680	1,4-Dichlorobenzene-d4	6.89

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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Data File : BF118003.D
Acq On : 26 Nov 2019 13:28
Operator : JU
Sample : PB125092BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB125092BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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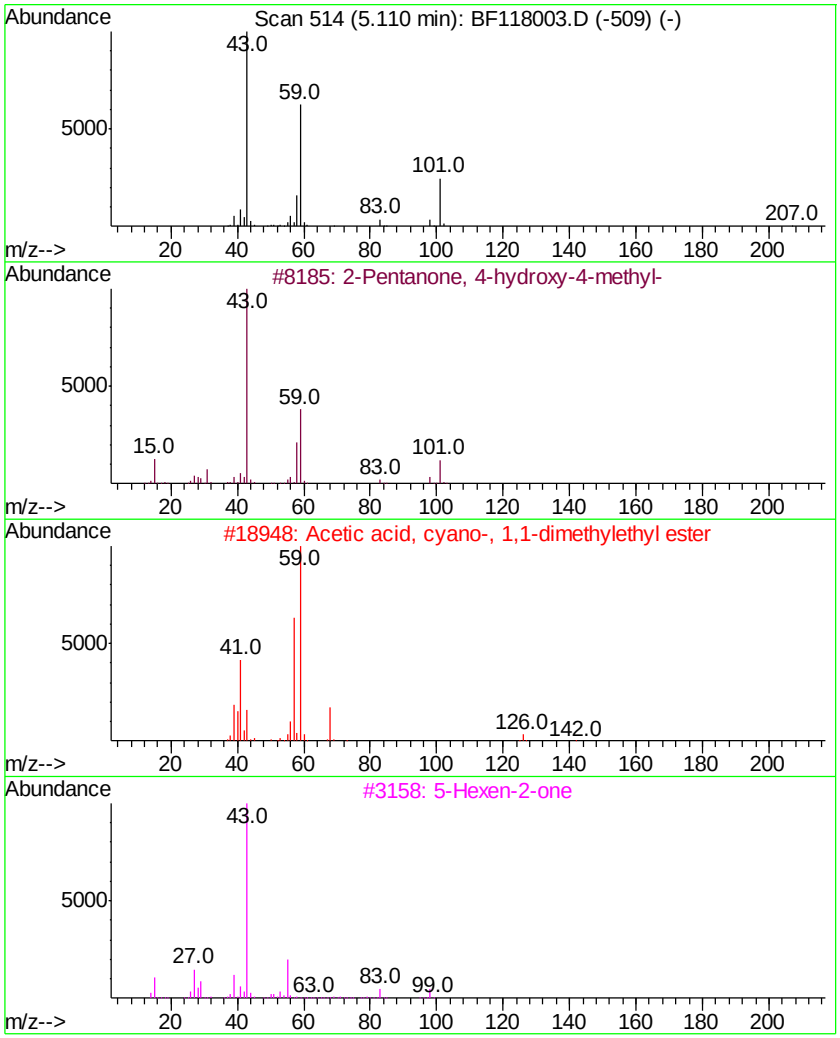
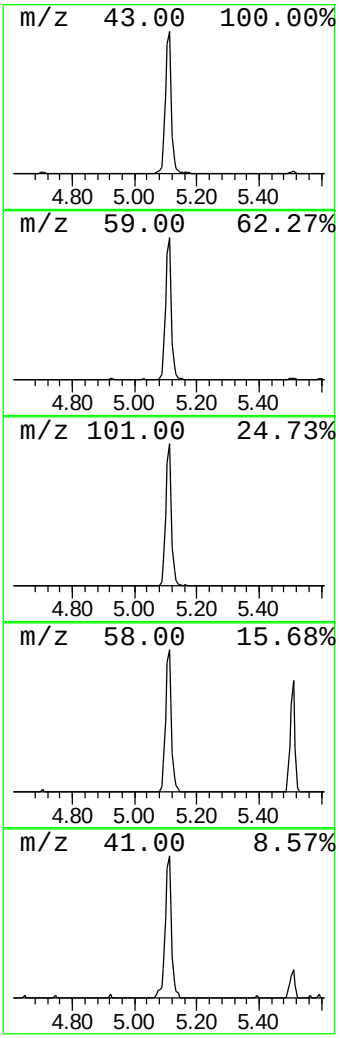
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	10.68 ng	506384	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
Data File : BF118003.D
Acq On : 26 Nov 2019 13:28
Operator : JU
Sample : PB125092BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB125092BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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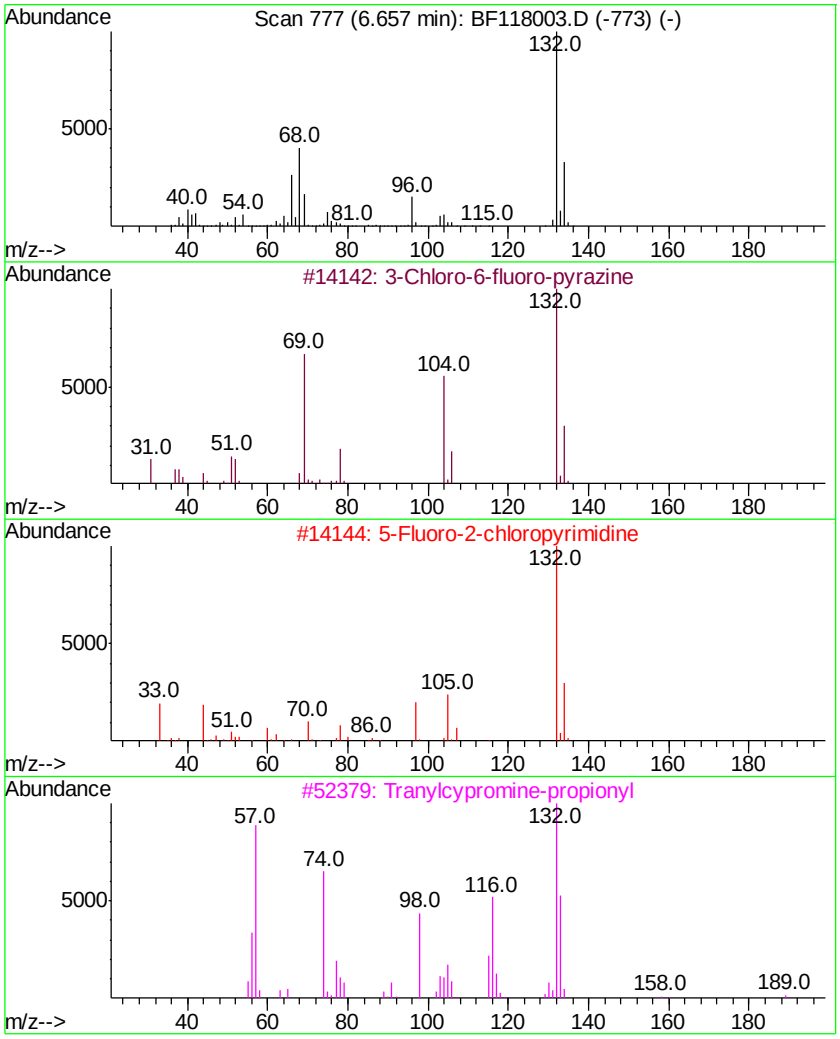
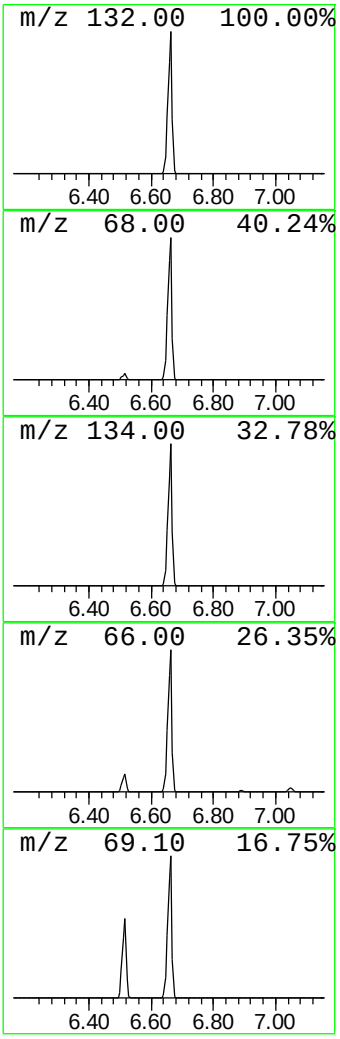
Peak Number 3 unknown6.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	91.49 ng	4336600	1,4-Dichlorobenzene-d4	6.89

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	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
Data File : BF118003.D
Acq On : 26 Nov 2019 13:28
Operator : JU
Sample : PB125092BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB125092BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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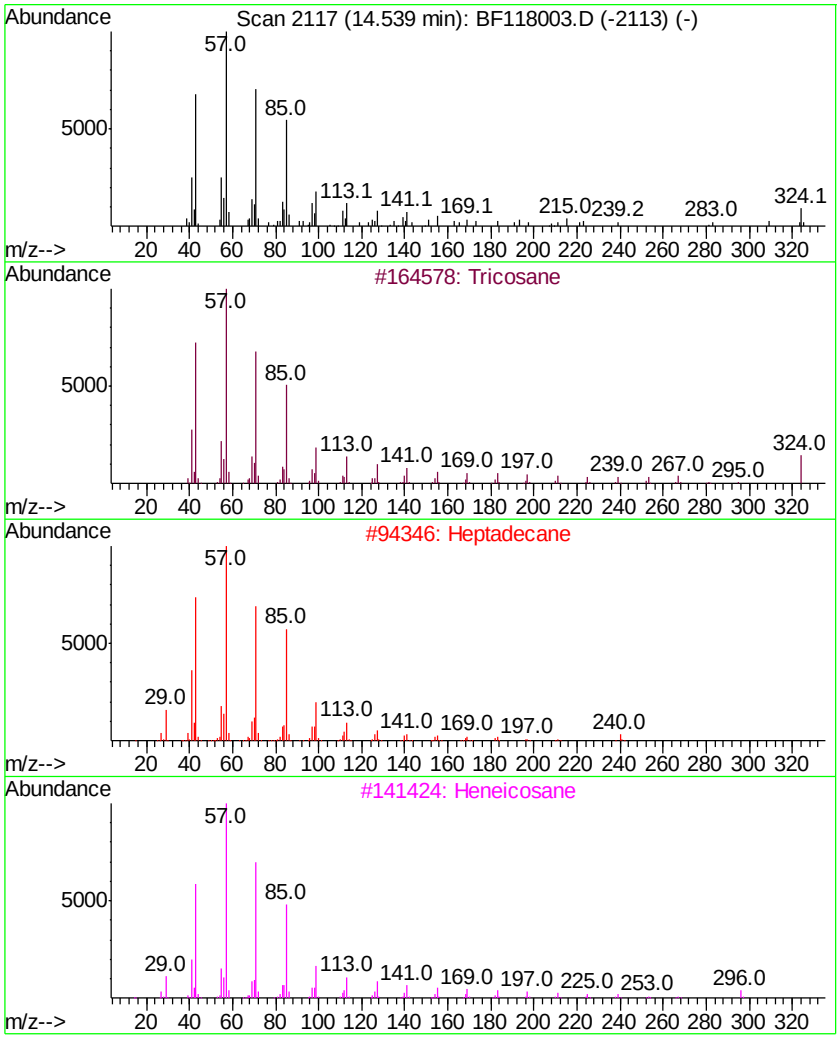
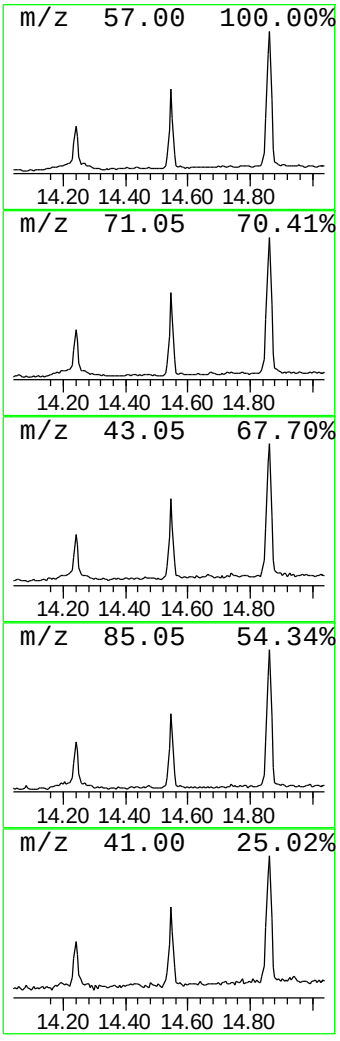
Peak Number 5 Tricosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	2.69 ng	179112	Chrysene-d12	14.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	95
2	Heptadecane	240	C17H36	000629-78-7	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Triacontane	422	C30H62	000638-68-6	90
5	Pentacosane	352	C25H52	000629-99-2	90





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Data File : BF118003.D
Acq On : 26 Nov 2019 13:28
Operator : JU
Sample : PB125092BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB125092BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

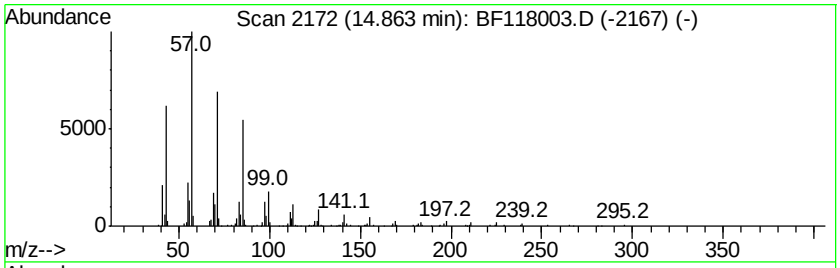
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

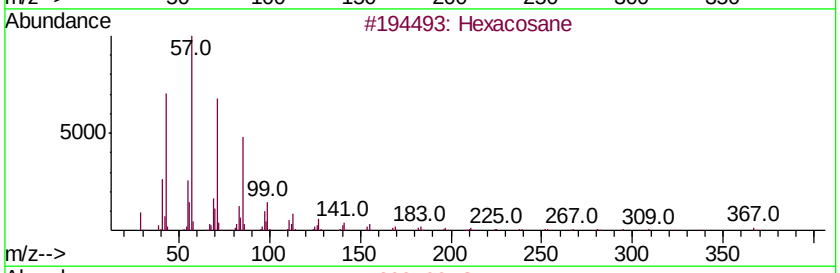
****

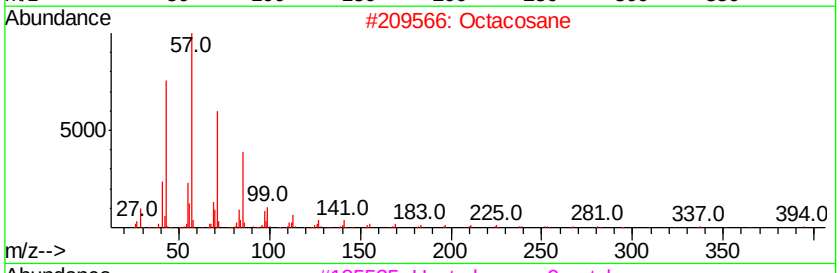
Peak Number 6 Hexacosane Concentration Rank 8

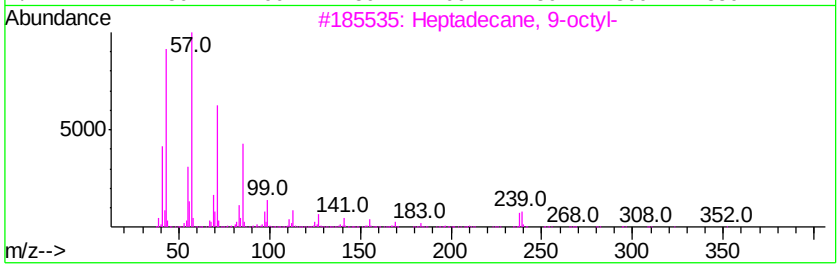
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	5.00 ng	310739	Perylene-d12	15.59

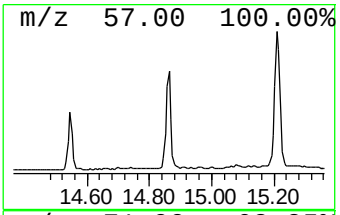
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Octacosane	394	C28H58	000630-02-4	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Tetracosane	338	C24H50	000646-31-1	91

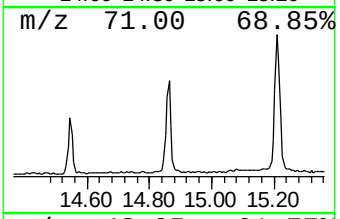


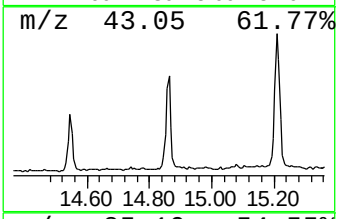


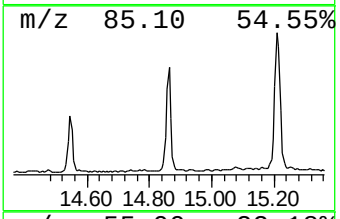


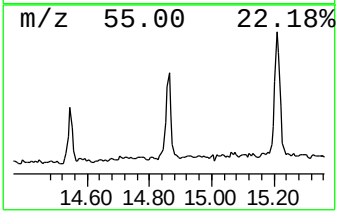












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
Data File : BF118003.D
Acq On : 26 Nov 2019 13:28
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB125092BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

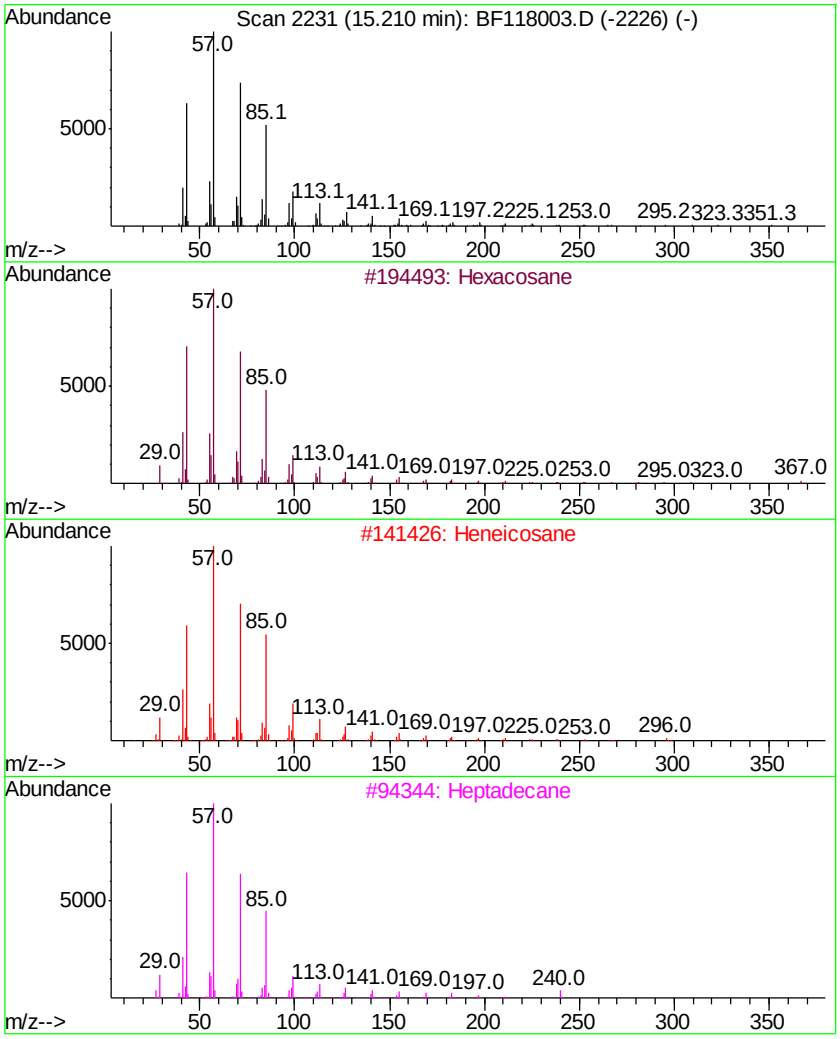
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

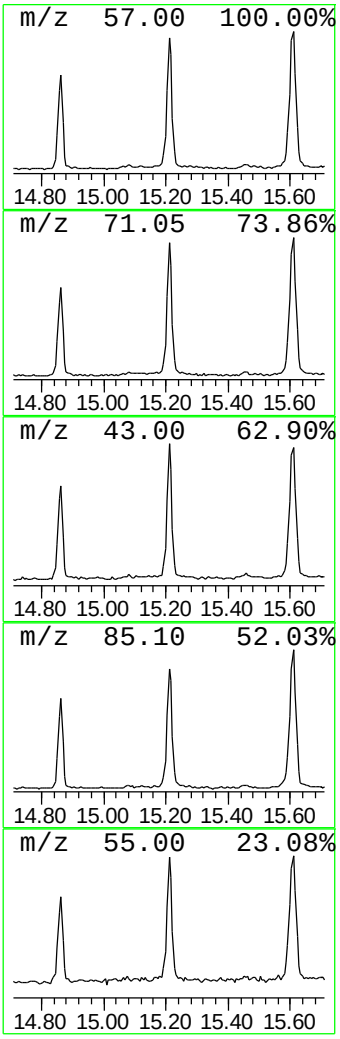
****

Peak Number 7 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.21	7.59 ng	471715	Perylene-d12	15.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
5	Triacontane	422	C30H62	000638-68-6	91





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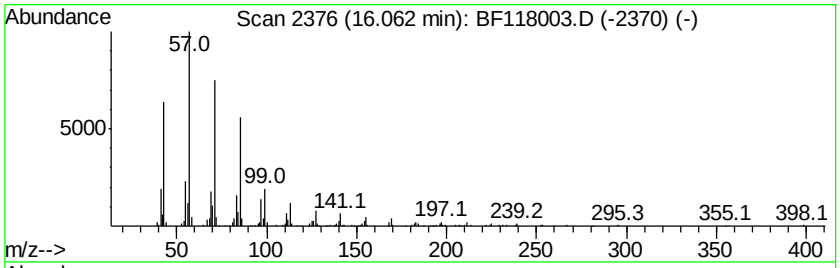
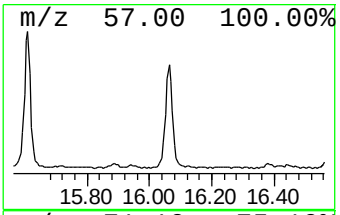
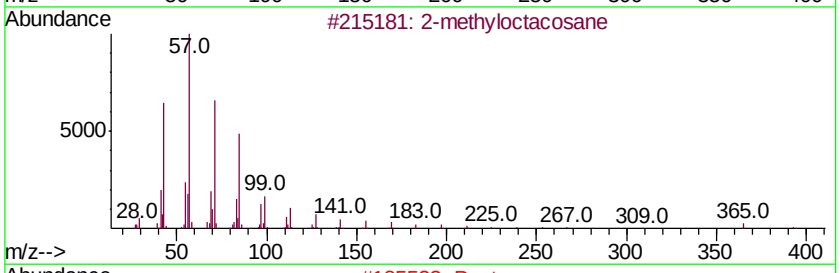
Peak Number 8 2-methyloctacosane Concentration Rank 5

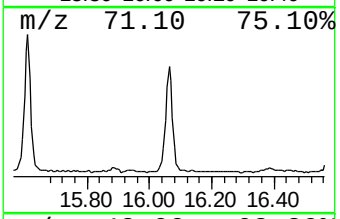
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.06	8.01 ng	498181	Perylene-d12	15.59

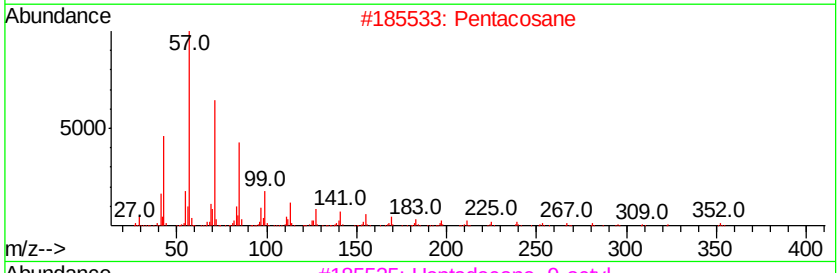
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Pentacosane	352	C25H52	000629-99-2	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Docosane	310	C22H46	000629-97-0	91
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90

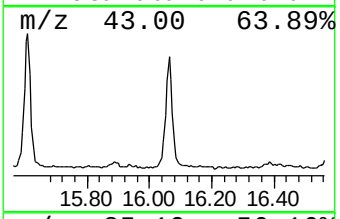


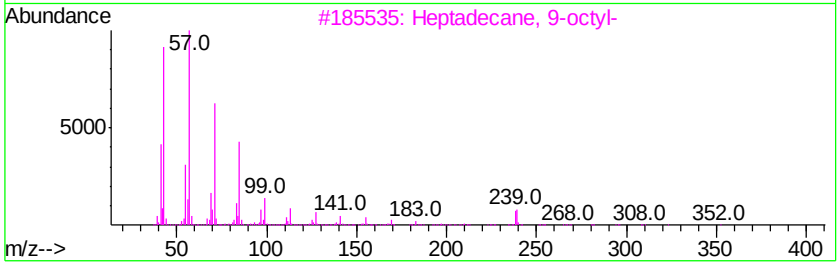


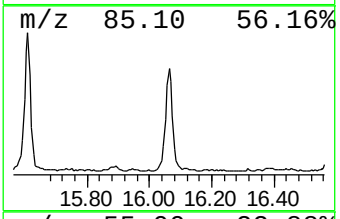


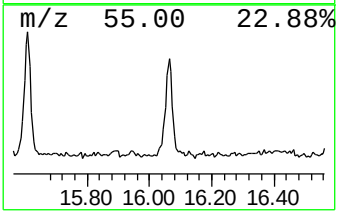












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
Data File : BF118003.D
Acq On : 26 Nov 2019 13:28
Operator : JU
Sample : PB125092BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB125092BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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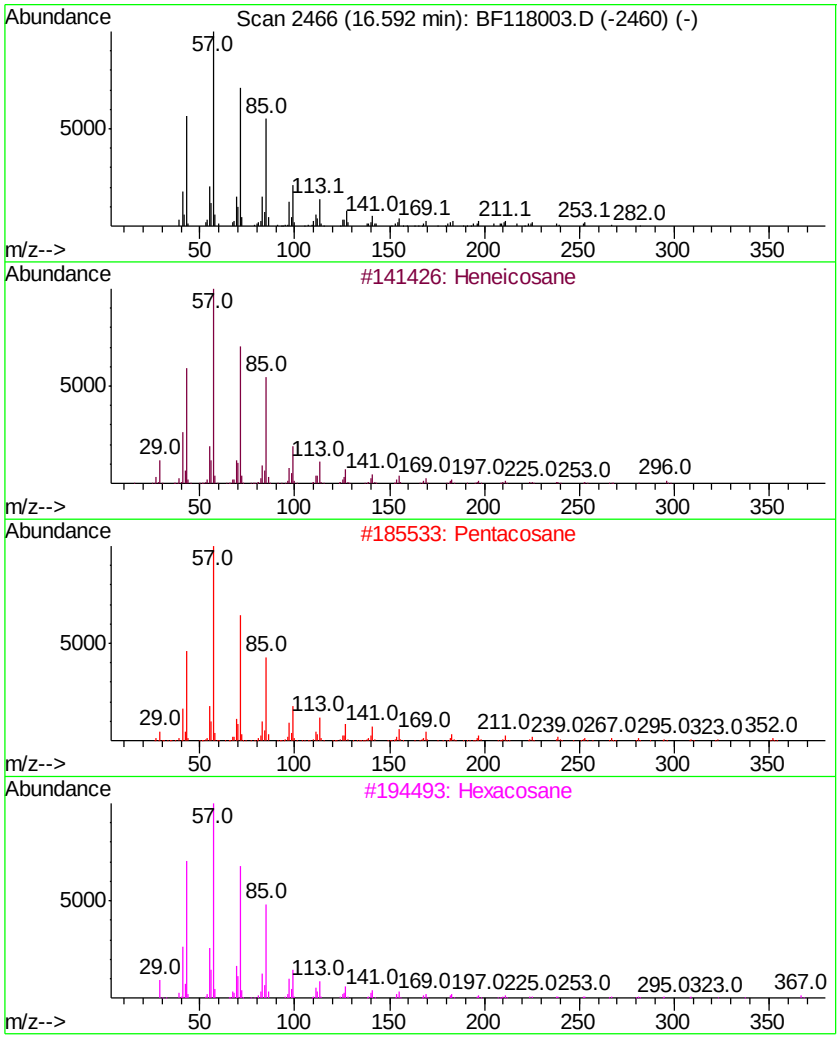
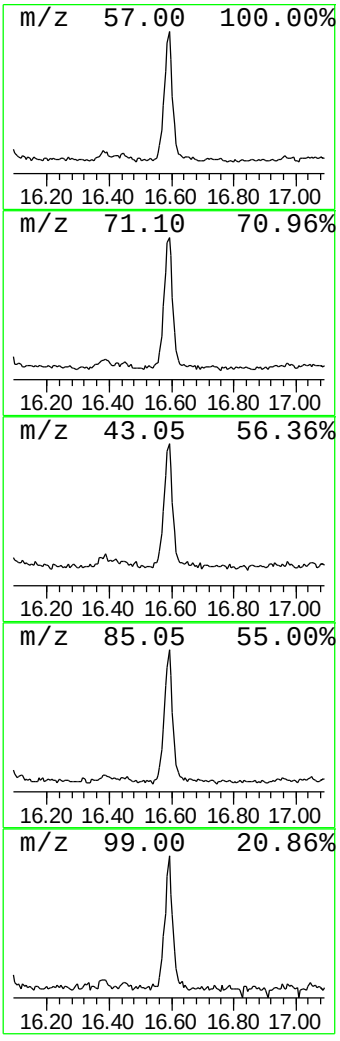
Peak Number 9 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.59	5.14 ng	319365	Perylene-d12	15.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Pentacosane	352	C25H52	000629-99-2	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Triacontane	422	C30H62	000638-68-6	83
5	Tetracosane	338	C24H50	000646-31-1	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112619\
Data File : BF118003.D
Acq On : 26 Nov 2019 13:28
Operator : JU
Sample : PB125092BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB125092BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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
Butane, 2-methoxy...	2.20	115.2	ng	5458680	1	6.89	948042	20.0
2-Pentanone, 4-hy...	5.11	10.7	ng	506384	1	6.89	948042	20.0
unknown6.66	6.66	91.5	ng	4336600	1	6.89	948042	20.0
Tricosane	14.54	2.7	ng	179112	5	14.08	1331130	20.0
Hexacosane	14.86	5.0	ng	310739	6	15.59	1243520	20.0
Heptadecane	15.21	7.6	ng	471715	6	15.59	1243520	20.0
2-methyloctacosane	16.06	8.0	ng	498181	6	15.59	1243520	20.0
Pentacosane	16.59	5.1	ng	319365	6	15.59	1243520	20.0