

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072718\
 Data File : BF107745.D
 Acq On : 27 Jul 2018 14:59
 Operator : JU/SJ
 Sample : J4180-05
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GS-PIT-2

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BF072018.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	5.195	482	486	501	rBV	280944	404887	12.96%	1.297%
2	5.595	551	554	584	rBV	1274203	2399586	76.79%	7.686%
3	6.595	721	724	744	rBV	1397566	2577001	82.47%	8.254%
4	6.731	744	747	770	rVB	2000336	2872920	91.94%	9.202%
5	6.960	783	786	808	rBV	437989	854649	27.35%	2.737%
6	7.113	808	812	837	rVB	1748169	2139644	68.47%	6.853%
7	7.525	879	882	906	rBV	948049	1729444	55.34%	5.539%
8	8.242	1000	1004	1025	rBV	822617	1210726	38.74%	3.878%
9	9.313	1182	1186	1203	rBV	2669459	3124930	100.00%	10.009%
10	9.707	1248	1253	1260	rBV	144147	191248	6.12%	0.613%
11	10.001	1299	1303	1322	rVB	1098116	1303756	41.72%	4.176%
12	10.795	1434	1438	1450	rBV	1449918	2013656	64.44%	6.450%
13	10.877	1450	1452	1463	rVB5	43510	101535	3.25%	0.325%
14	11.495	1553	1557	1569	rBV	981989	1360113	43.52%	4.356%
15	11.830	1611	1614	1622	rVB2	25733	44176	1.41%	0.141%
16	12.001	1639	1643	1646	rBV	212118	235710	7.54%	0.755%
17	12.113	1659	1662	1668	rVB2	32293	56868	1.82%	0.182%
18	12.548	1733	1736	1739	rBV2	29336	37696	1.21%	0.121%
19	12.713	1760	1764	1772	rBV	118339	188362	6.03%	0.603%
20	12.783	1773	1776	1786	rVV5	75054	134932	4.32%	0.432%
21	12.942	1798	1803	1809	rBV	167822	242515	7.76%	0.777%
22	13.077	1822	1826	1836	rBV	2372840	2587183	82.79%	8.287%
23	13.624	1916	1919	1921	rBV3	40043	45759	1.46%	0.147%
24	13.954	1972	1975	1980	rBV2	161030	171625	5.49%	0.550%
25	14.142	2003	2007	2019	rBV	906671	1281359	41.00%	4.104%
26	14.271	2027	2029	2032	rVB	66498	55056	1.76%	0.176%
27	14.577	2078	2081	2087	rVB	182764	190591	6.10%	0.610%
28	14.895	2131	2135	2140	rBV	358932	384512	12.30%	1.232%
29	15.248	2192	2195	2200	rVB	529504	646024	20.67%	2.069%
30	15.654	2259	2264	2265	rBV	510059	676766	21.66%	2.168%
31	15.671	2265	2267	2283	rVB2	662327	1094016	35.01%	3.504%
32	16.107	2337	2341	2348	rVB	360835	574318	18.38%	1.840%
33	16.648	2429	2433	2439	rVB	168206	288945	9.25%	0.925%

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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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-BF072018.M
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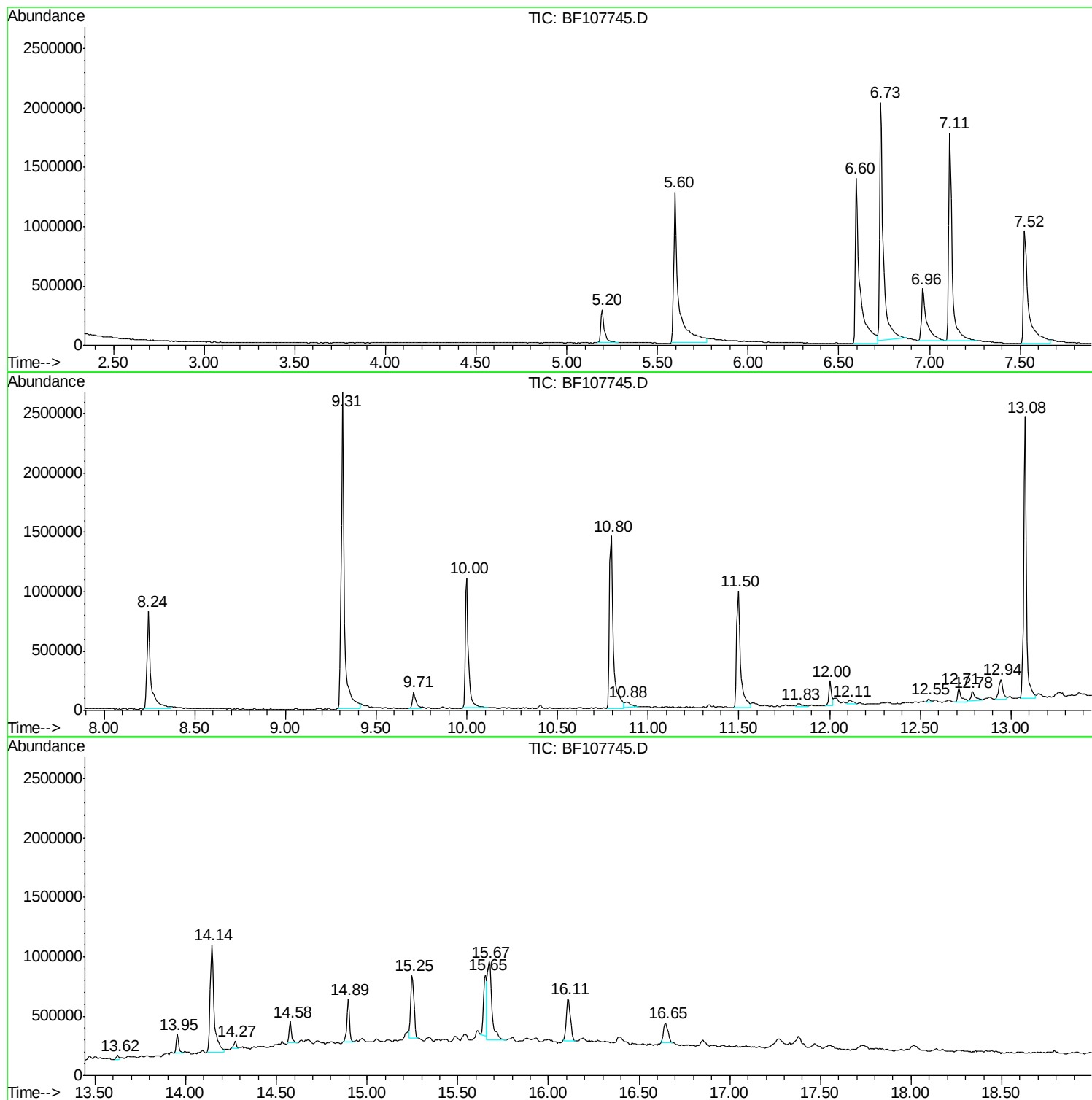
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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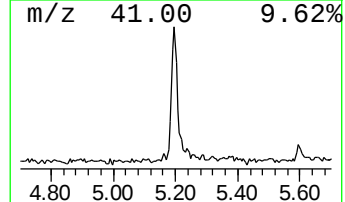
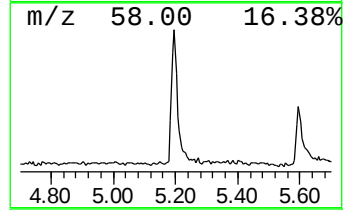
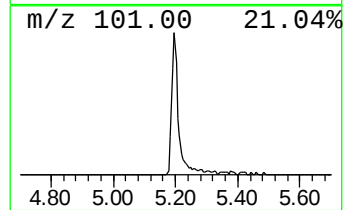
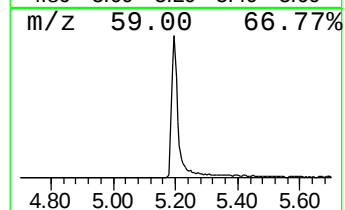
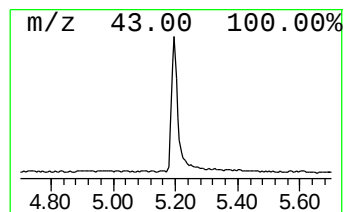
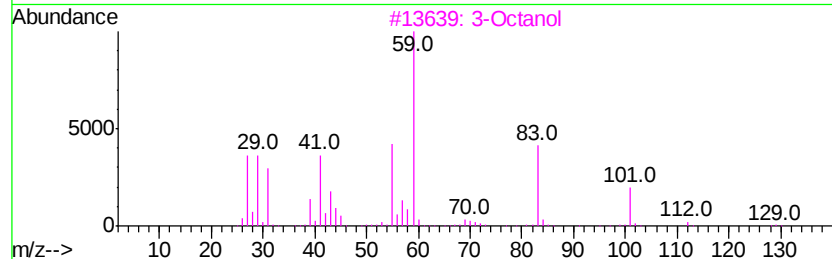
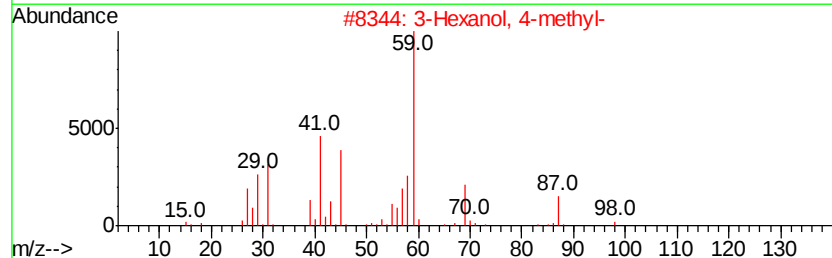
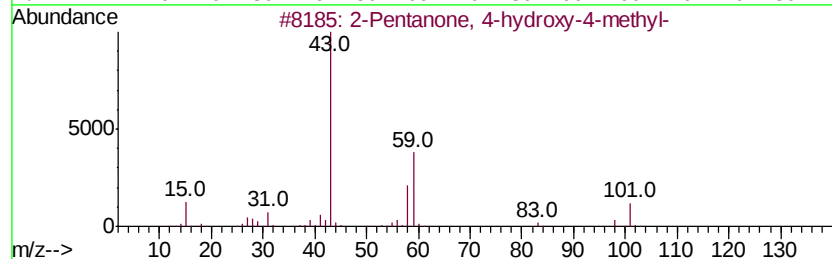
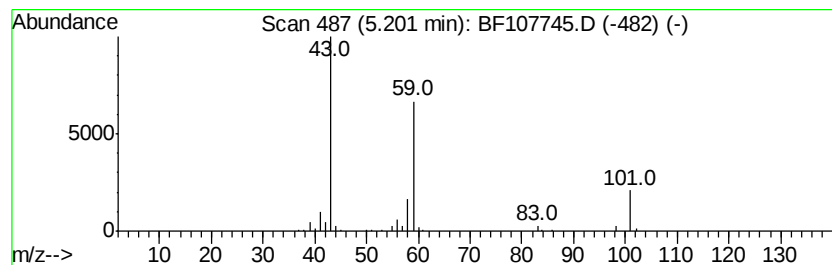
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	9.47 ng	404887	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			3-Octanol	130	C8H18O	000589-98-0	33
4			Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	32
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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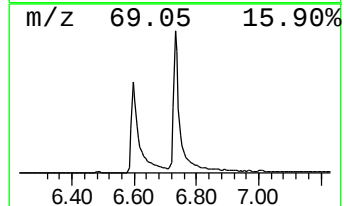
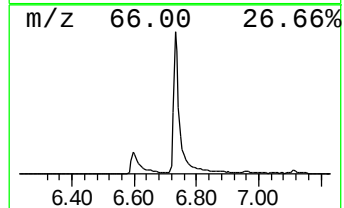
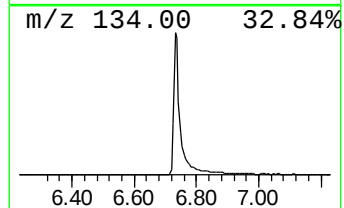
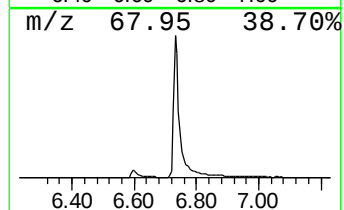
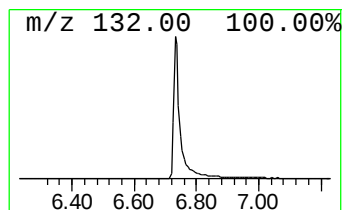
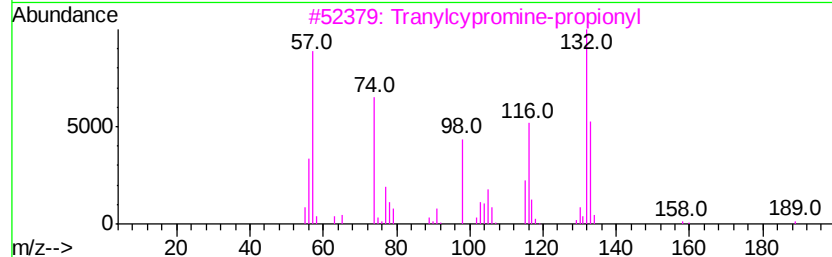
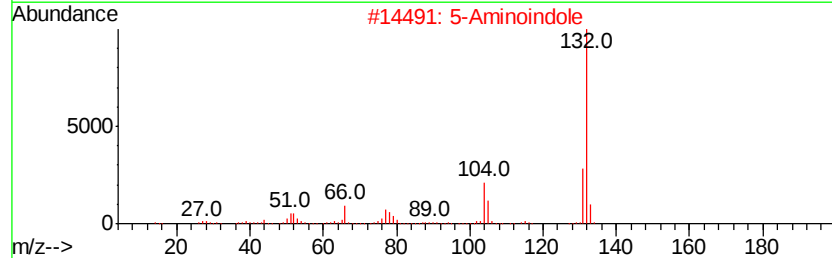
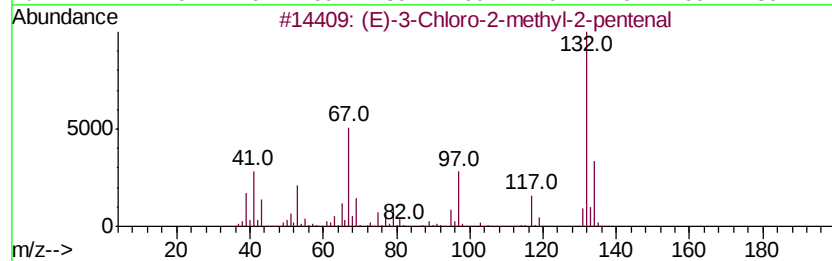
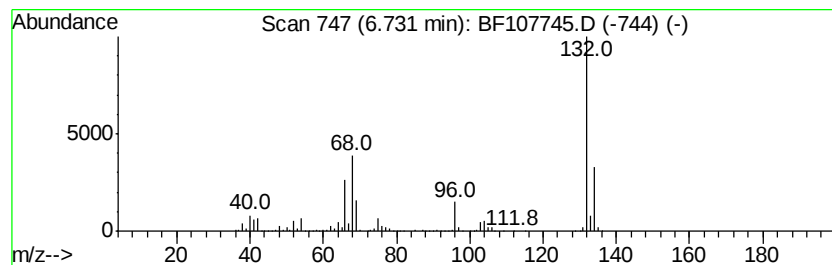
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	67.23 ng	2872920	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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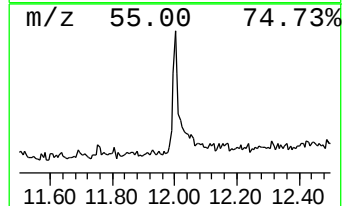
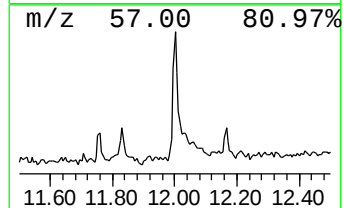
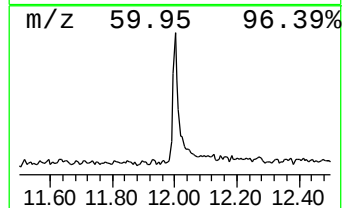
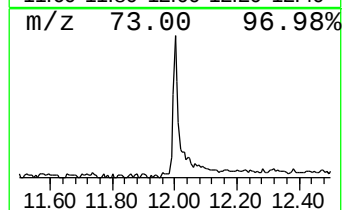
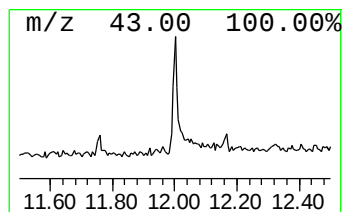
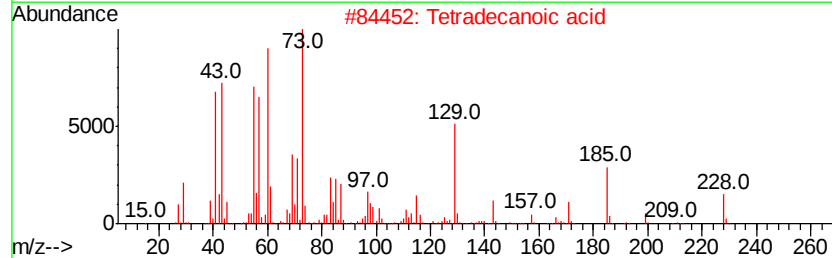
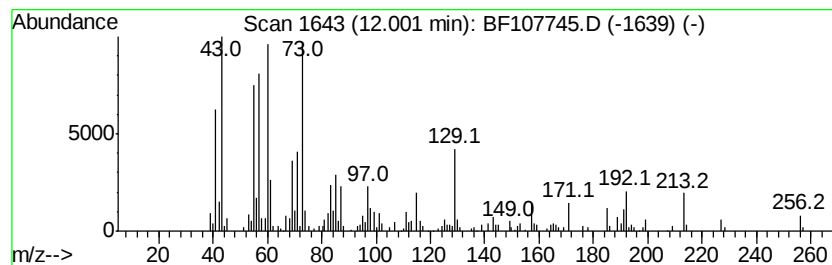
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	3.47 ng	235710	Phenanthrene-d10	11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	92
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		Tridecanoic acid	214	C13H26O2	000638-53-9	86
5		Nonanoic acid	158	C9H18O2	000112-05-0	38



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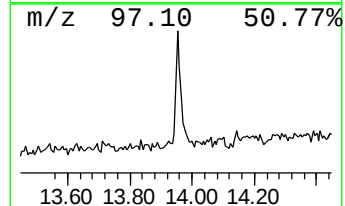
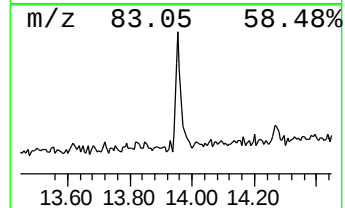
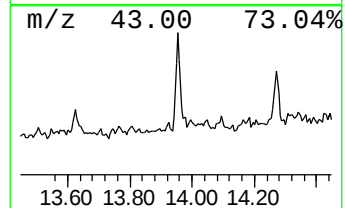
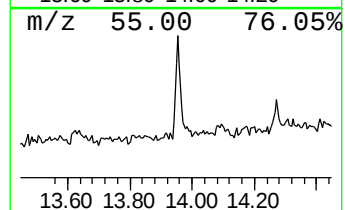
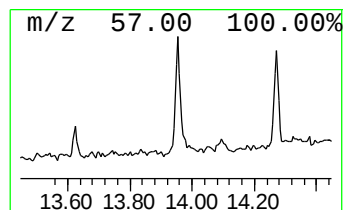
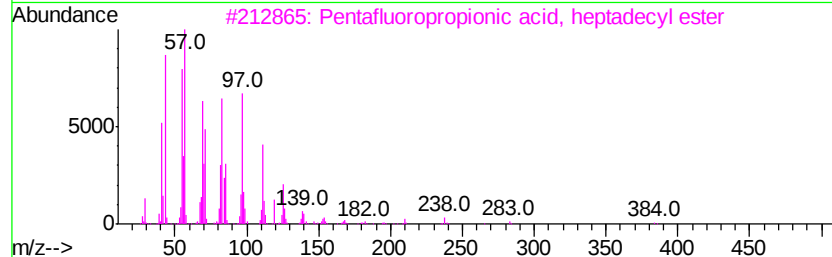
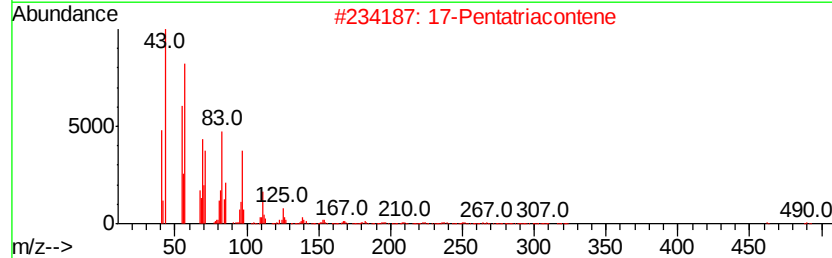
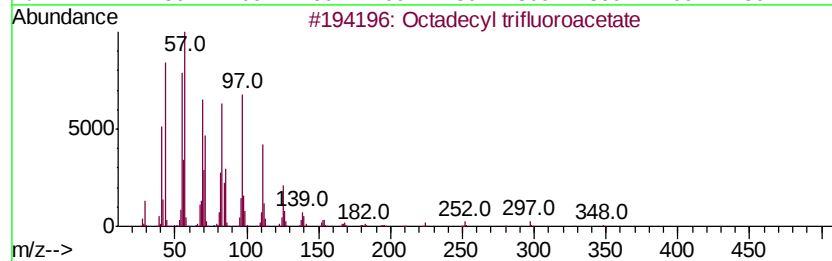
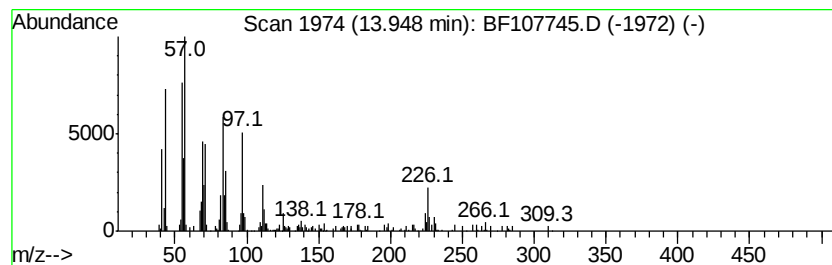
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecyl trifluoroacetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	2.68 ng	171625	Chrysene-d12	14.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
2		17-Pentatriacontene	491	C35H70	006971-40-0	90
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	87
4		Z-5-Nonadecene	266	C19H38	1000131-11-8	87
5		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	86



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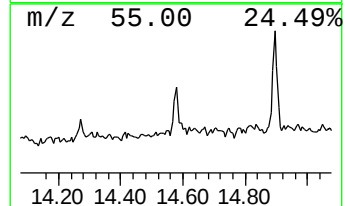
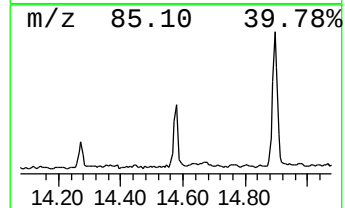
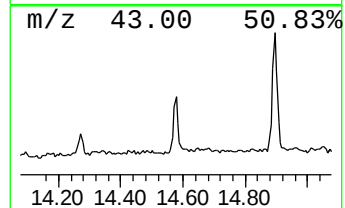
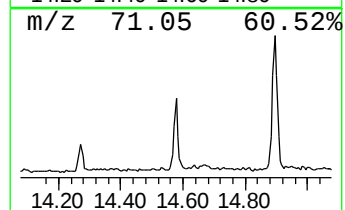
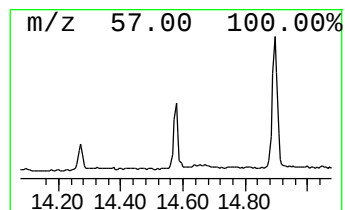
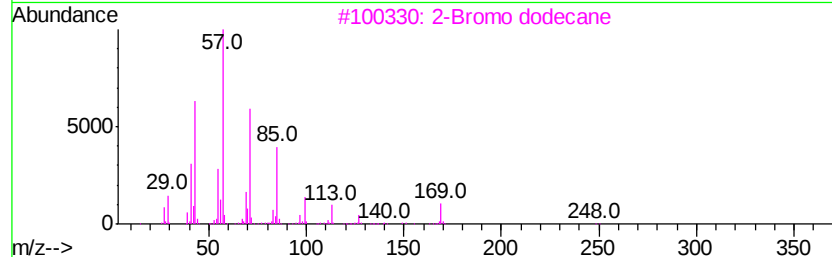
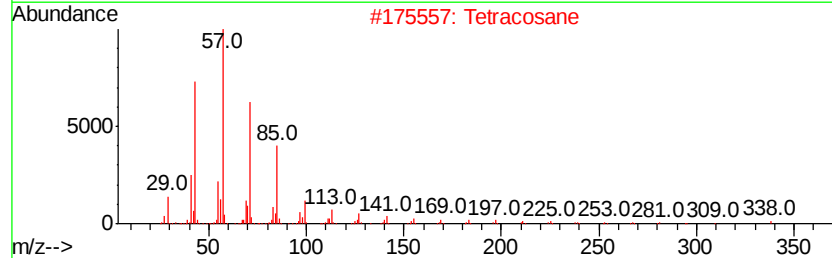
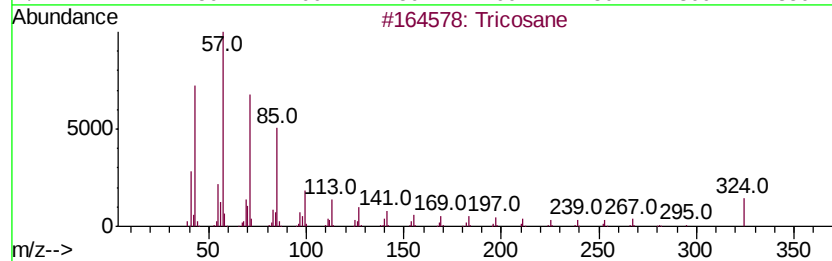
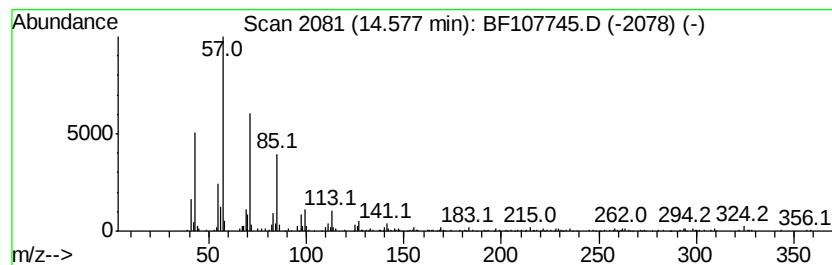
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tricosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	2.97 ng	190591	Chrysene-d12	14.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane		324	C23H48	000638-67-5	93
2	Tetracosane		338	C24H50	000646-31-1	90
3	2-Bromo dodecane		248	C12H25Br	013187-99-0	90
4	Heptacosane		380	C27H56	000593-49-7	90
5	Octacosane		394	C28H58	000630-02-4	90



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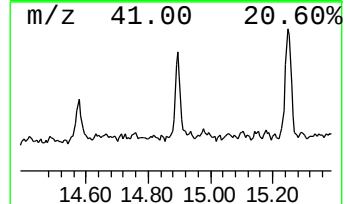
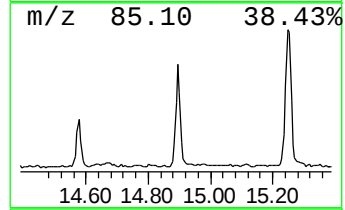
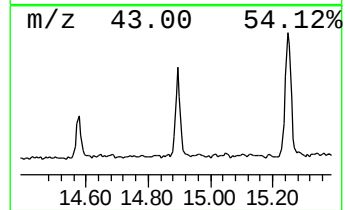
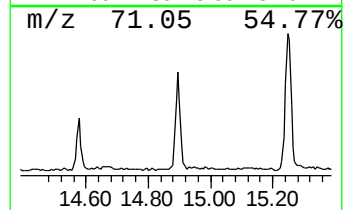
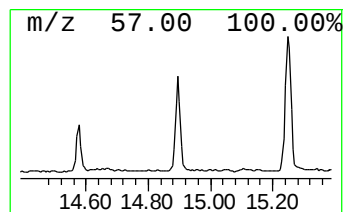
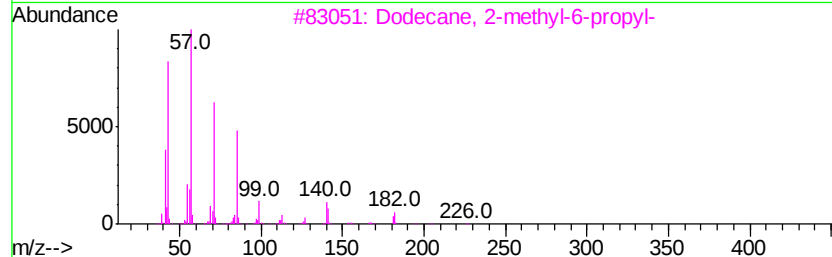
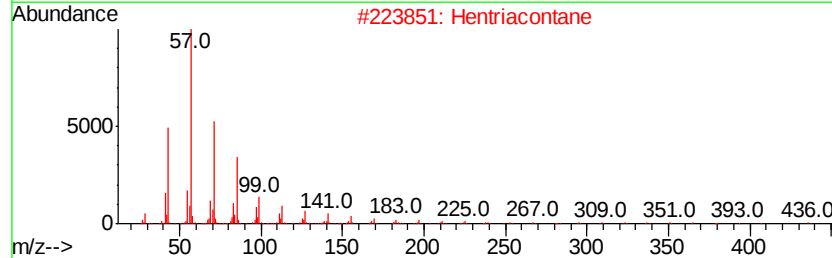
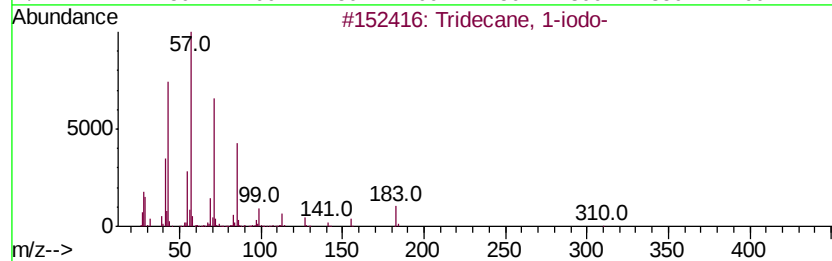
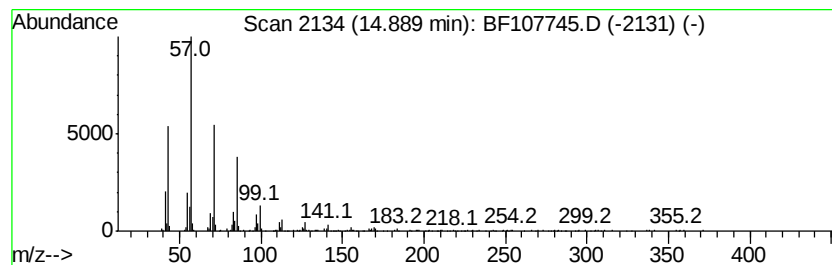
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tridecane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	6.00 ng	384512	Chrysene-d12	14.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	93
2		Hentriacontane	437	C31H64	000630-04-6	91
3		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	87
4		Tetradecane, 4-ethyl-	226	C16H34	055045-14-2	83
5		Tetracosane	338	C24H50	000646-31-1	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072718\
Data File : BF107745.D
Acq On : 27 Jul 2018 14:59
Operator : JU/SJ
Sample : J4180-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GS-PIT-2

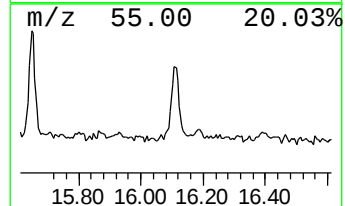
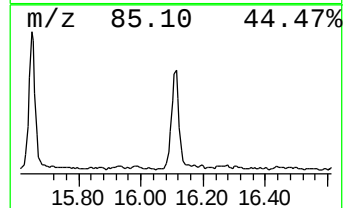
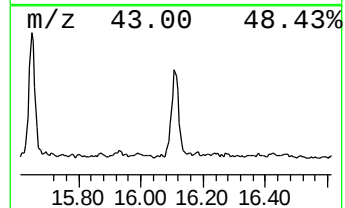
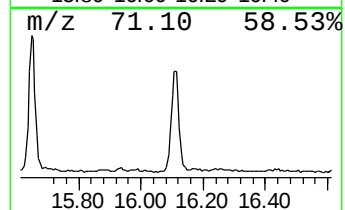
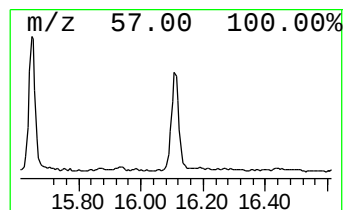
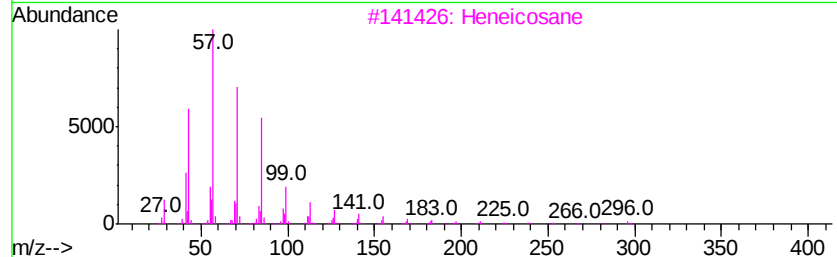
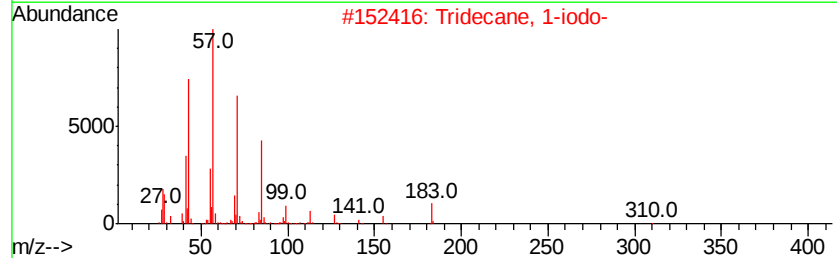
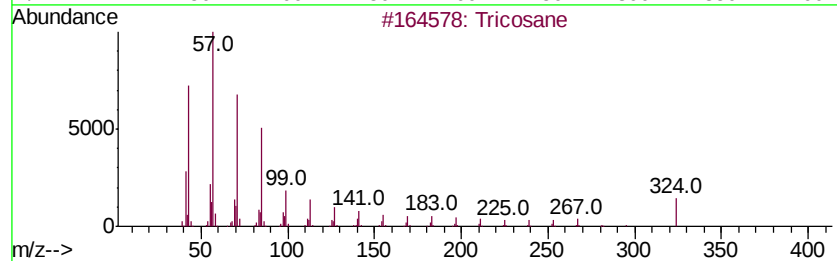
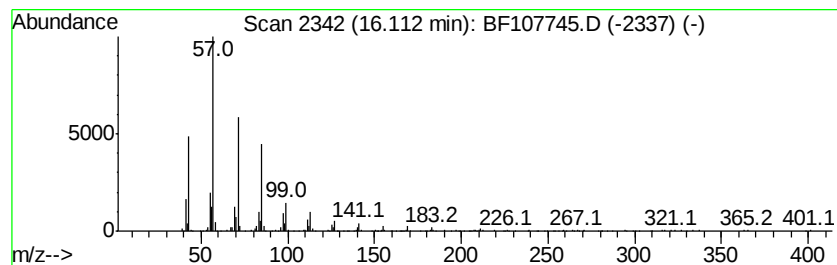
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.11	10.50 ng	574318	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tricosane	324	C23H48	000638-67-5	91
2		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Heptacosane	380	C27H56	000593-49-7	87
5		Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072718\
Data File : BF107745.D
Acq On : 27 Jul 2018 14:59
Operator : JU/SJ
Sample : J4180-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GS-PIT-2

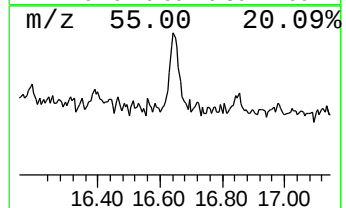
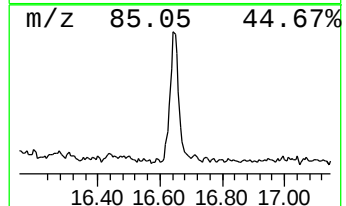
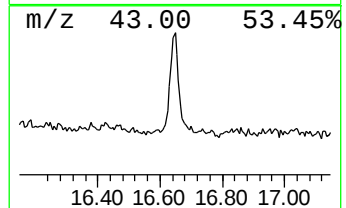
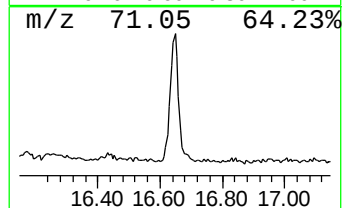
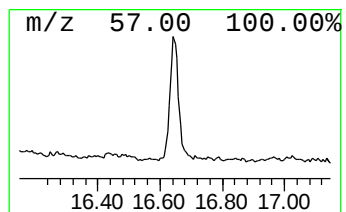
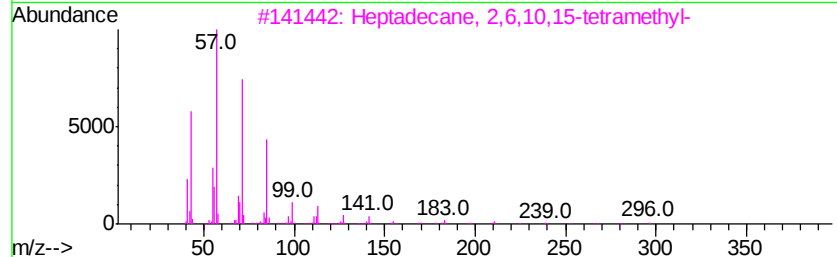
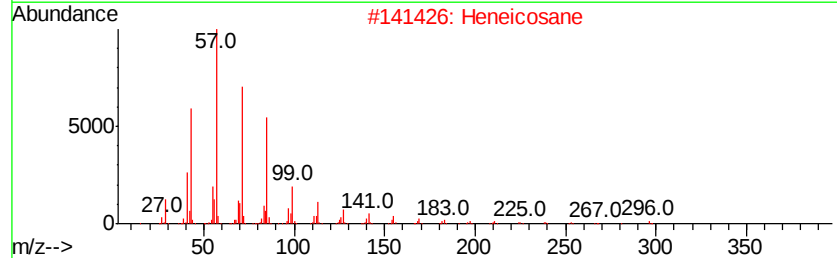
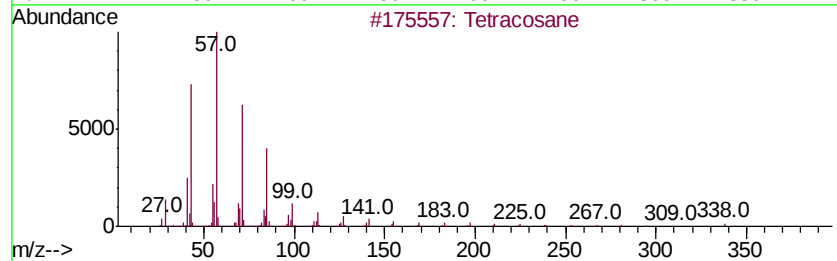
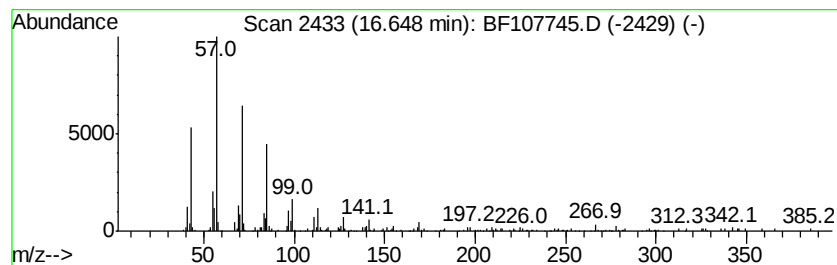
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.65	5.28 ng	288945	Perylene-d12	15.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	96
2		Heneicosane	296	C21H44	000629-94-7	95
3		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
4		Tricosane, 2-methyl-	338	C24H50	001928-30-9	90
5		Tetratetracontane	619	C44H90	007098-22-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072718\
Data File : BF107745.D
Acq On : 27 Jul 2018 14:59
Operator : JU/SJ
Sample : J4180-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GS-PIT-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.20	9.5	ng	404887	1	6.96	854649	20.0
unknown6.73	6.73	67.2	ng	2872920	1	6.96	854649	20.0
n-Hexadecanoic acid	12.00	3.5	ng	235710	4	11.50	1360110	20.0
Octadecyl trifluo...	13.95	2.7	ng	171625	5	14.14	1281360	20.0
Tricosane	14.58	3.0	ng	190591	5	14.14	1281360	20.0
Tridecane, 1-iodo-	14.89	6.0	ng	384512	5	14.14	1281360	20.0
Heneicosane	16.11	10.5	ng	574318	6	15.67	1094020	20.0
Tetracosane	16.65	5.3	ng	288945	6	15.67	1094020	20.0