

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100418\
 Data File : BF109605.D
 Acq On : 4 Oct 2018 23:22
 Operator : JU/SJ
 Sample : J5237-05
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BSS-GW1

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-BF092218.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	4.887	473	476	485	rBV	40026	51913	2.33%	0.328%
2	5.328	547	551	568	rBV	869167	928853	41.66%	5.866%
3	6.351	722	725	742	rBV	526994	663723	29.77%	4.191%
4	6.481	742	747	756	rBV	1541955	1612660	72.33%	10.184%
5	6.704	781	785	794	rBV	504356	478866	21.48%	3.024%
6	6.775	794	797	803	rVV	32568	35927	1.61%	0.227%
7	6.857	807	811	829	rVB	1602281	1537421	68.95%	9.709%
8	7.269	876	881	894	rBV	1083664	1260565	56.53%	7.961%
9	7.981	999	1002	1006	rBV	640414	586252	26.29%	3.702%
10	8.010	1006	1007	1017	rVB3	33620	36429	1.63%	0.230%
11	8.210	1037	1041	1043	rBV	29806	25086	1.13%	0.158%
12	8.263	1047	1050	1056	rVB	26586	31778	1.43%	0.201%
13	8.392	1063	1072	1081	rBV	180145	249642	11.20%	1.577%
14	9.057	1181	1185	1197	rBV	2301760	2229712	100.00%	14.081%
15	9.180	1204	1206	1209	rVB	32634	29010	1.30%	0.183%
16	9.451	1248	1252	1258	rBV	460280	369941	16.59%	2.336%
17	9.733	1296	1300	1308	rVB	671853	618268	27.73%	3.904%
18	10.116	1361	1365	1367	rBV	33136	30413	1.36%	0.192%
19	10.522	1430	1434	1444	rVB	950292	1001563	44.92%	6.325%
20	11.210	1547	1551	1564	rVB	562619	506012	22.69%	3.196%
21	11.751	1639	1643	1647	rBV	173382	177576	7.96%	1.121%
22	12.527	1772	1775	1780	rBV2	61875	77449	3.47%	0.489%
23	12.792	1815	1820	1825	rBV	1651573	1510350	67.74%	9.538%
24	13.692	1970	1973	1982	rBV	148963	201543	9.04%	1.273%
25	13.839	1994	1998	2005	rVB	540883	546015	24.49%	3.448%
26	14.015	2025	2028	2032	rVB4	18664	23226	1.04%	0.147%
27	14.315	2077	2079	2083	rBV3	35542	38871	1.74%	0.245%
28	14.610	2126	2129	2132	rVB	53254	46905	2.10%	0.296%
29	14.674	2138	2140	2144	rVB	44989	44975	2.02%	0.284%
30	14.921	2179	2182	2185	rBV	73405	80698	3.62%	0.510%
31	15.239	2232	2236	2240	rBV	434369	536947	24.08%	3.391%
32	15.274	2240	2242	2249	rVB	83985	90628	4.06%	0.572%
33	15.668	2305	2309	2314	rBV	73774	96930	4.35%	0.612%
34	16.127	2383	2387	2392	rBV	48002	78947	3.54%	0.499%

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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

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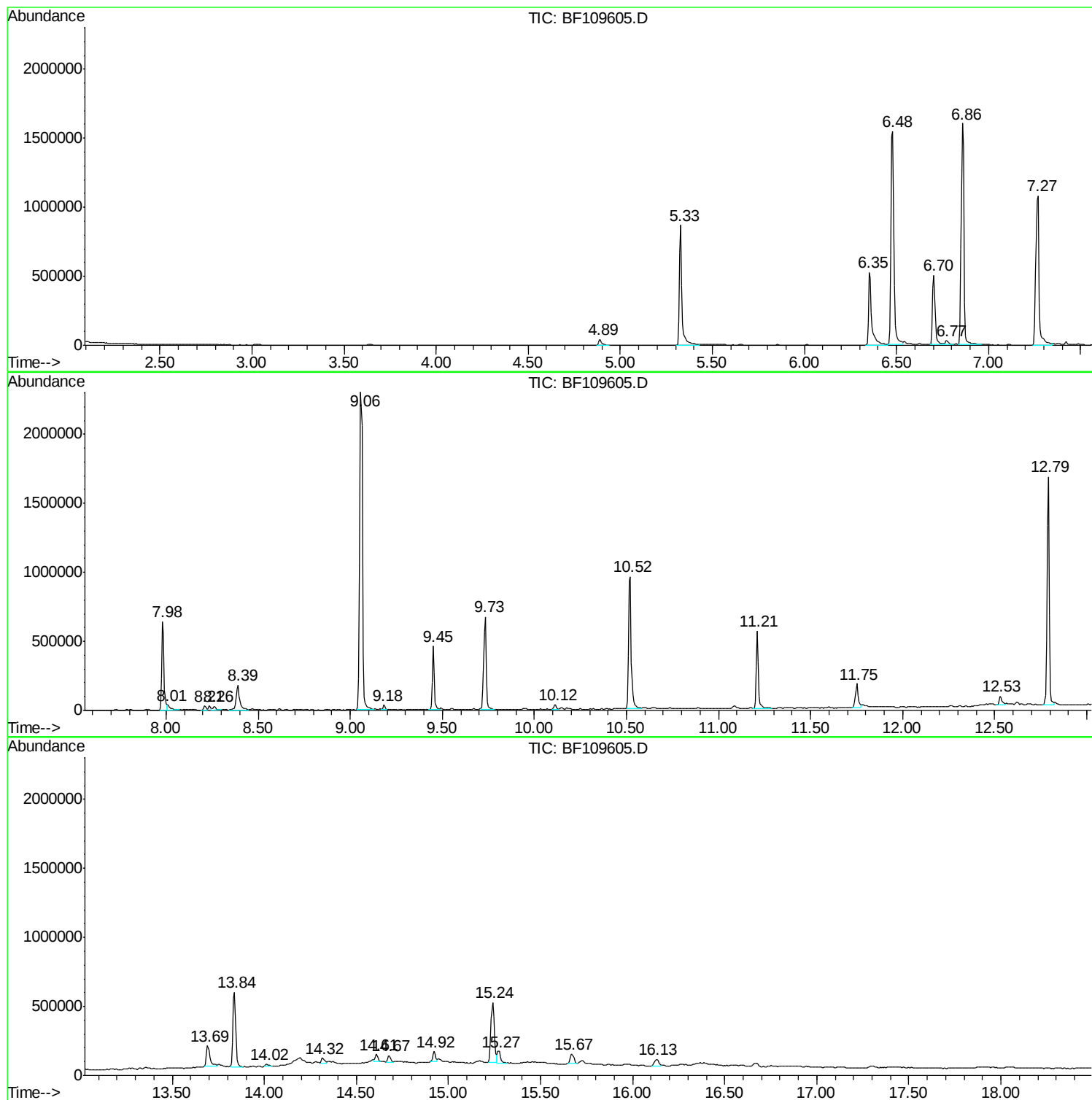
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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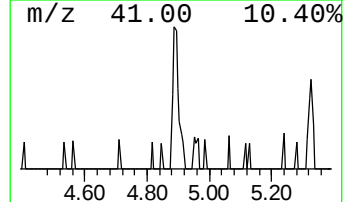
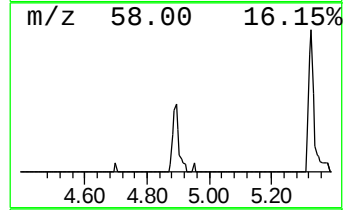
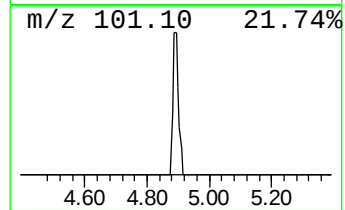
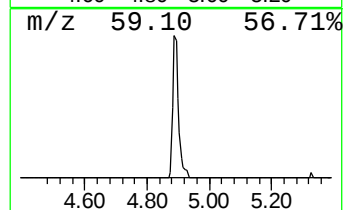
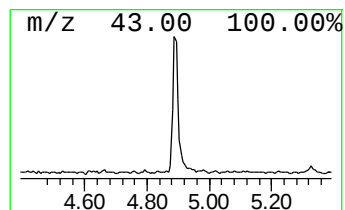
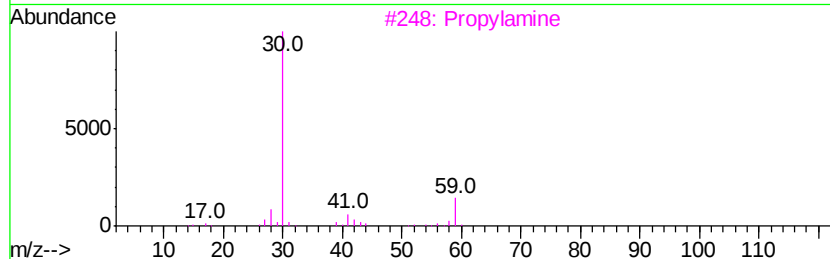
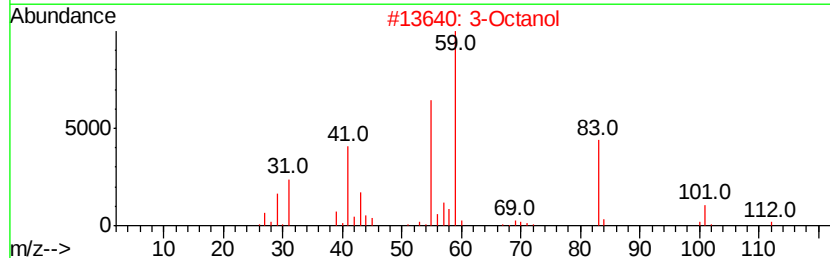
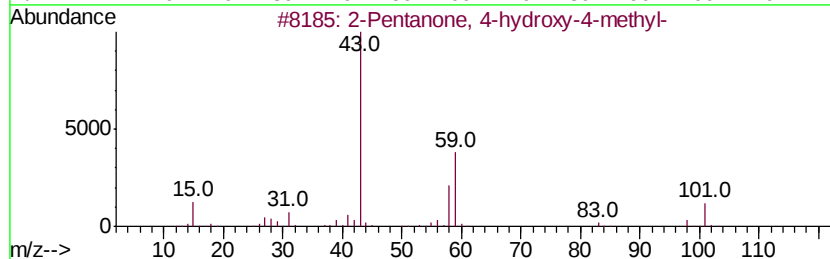
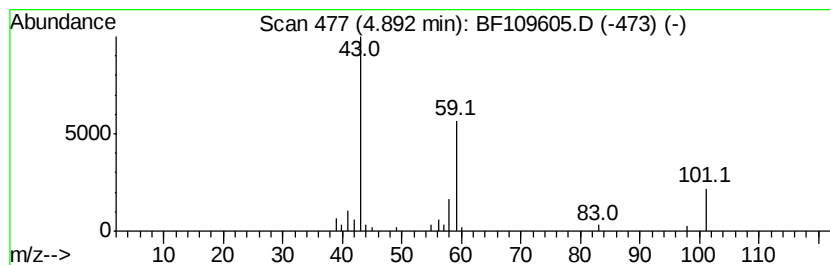
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	2.17 ng	51913	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	3-Octanol	130	C8H18O	000589-98-0	28
3	Propylamine	59	C3H9N	000107-10-8	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	3-Hexanol	102	C6H14O	000623-37-0	9



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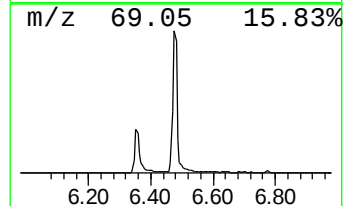
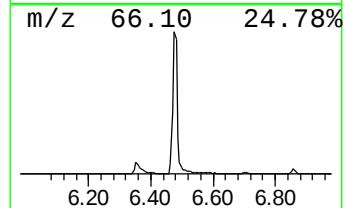
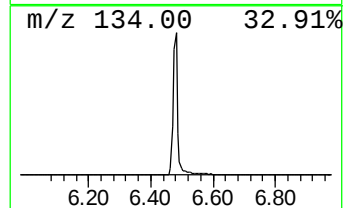
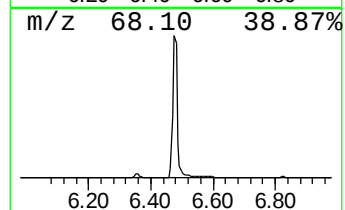
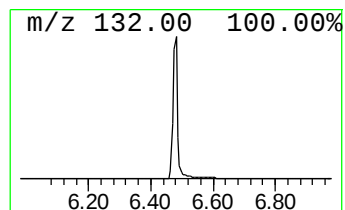
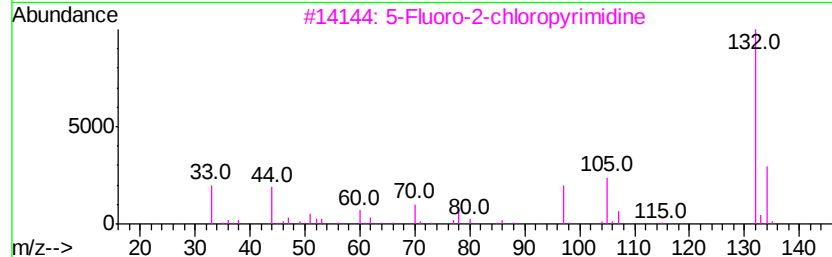
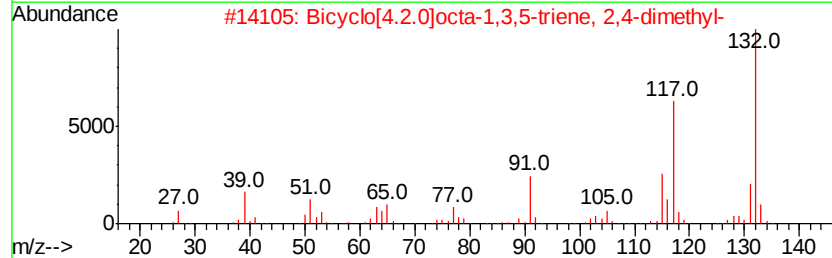
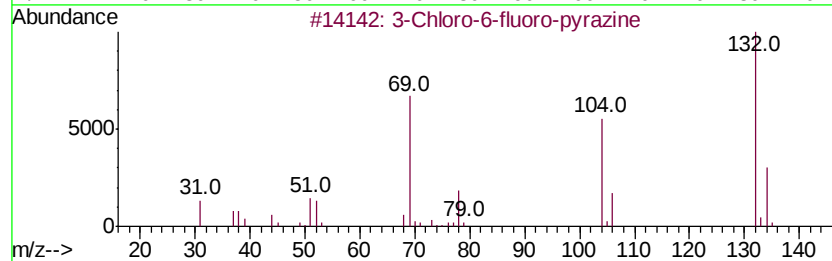
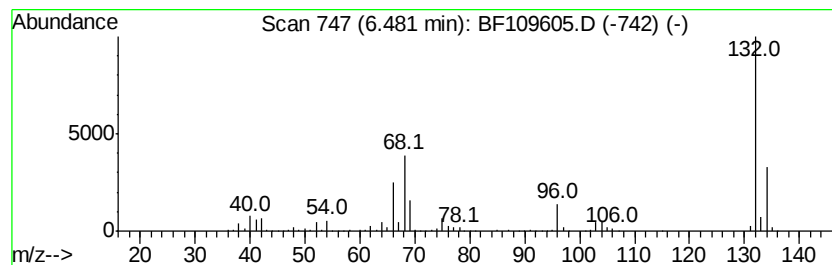
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	67.35 ng	1612660	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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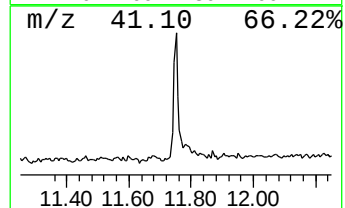
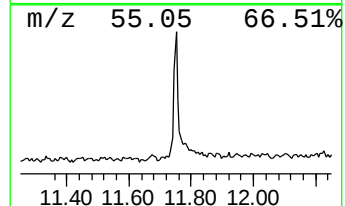
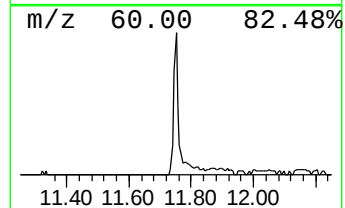
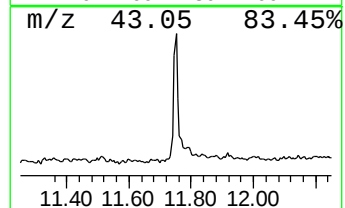
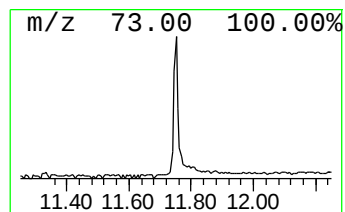
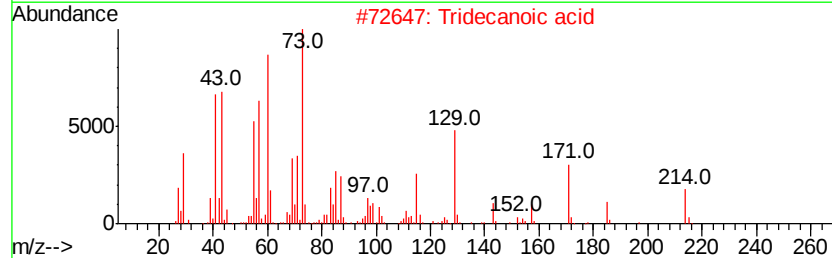
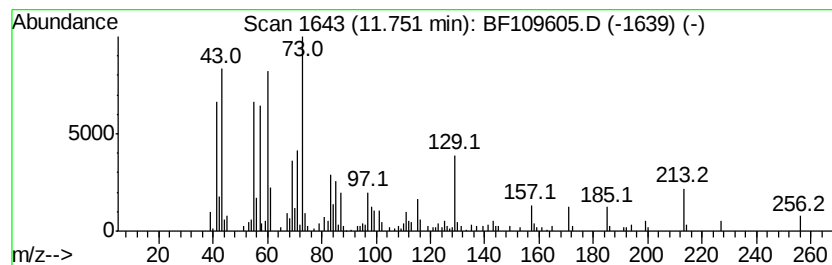
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	7.02 ng	177576	Phenanthrene-d10	11.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



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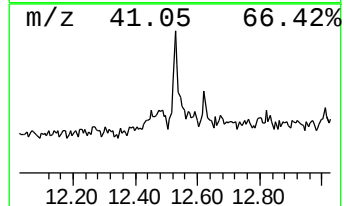
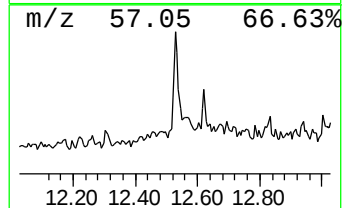
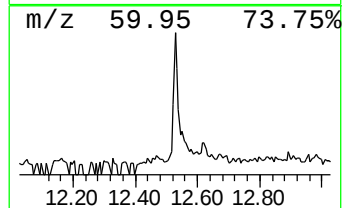
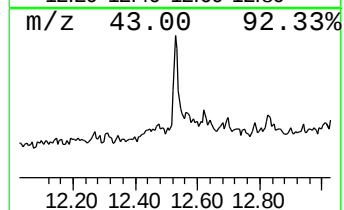
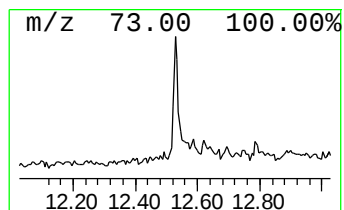
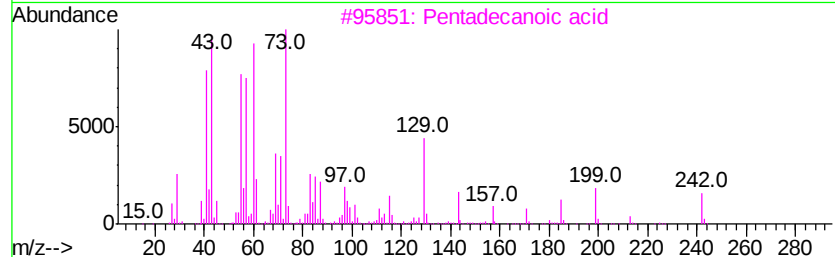
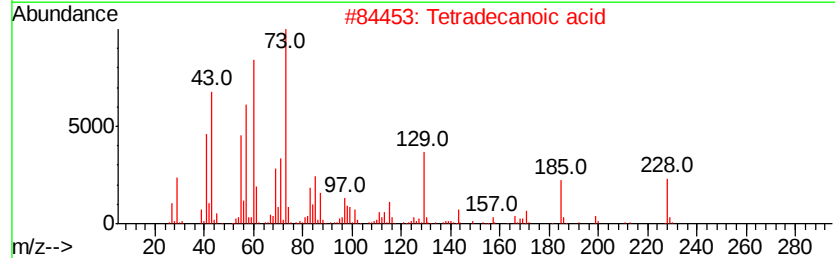
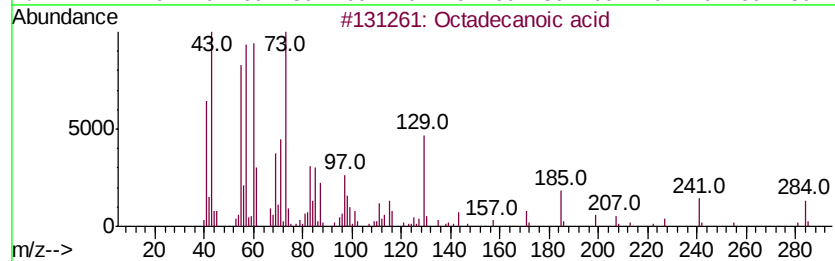
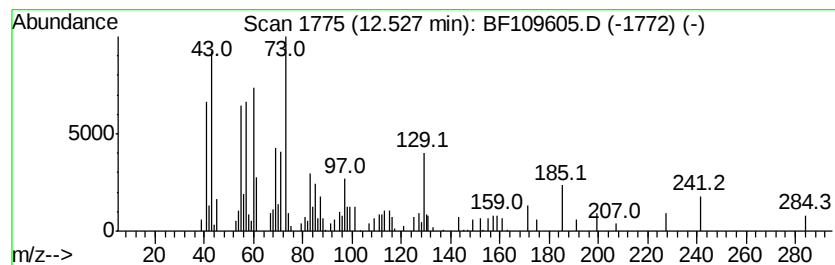
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.53	2.84 ng	77449	Chrysene-d12	13.84

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	59
5		Dodecanoic acid	200	C12H24O2	000143-07-7	53



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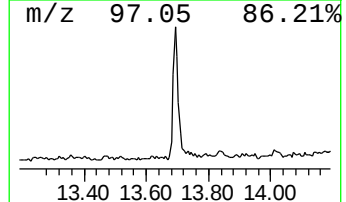
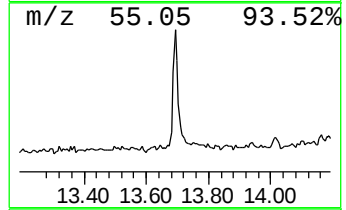
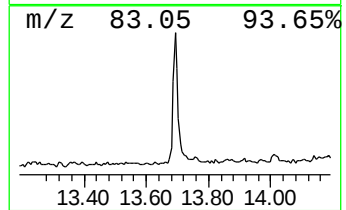
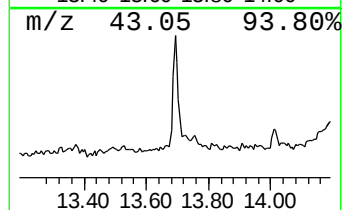
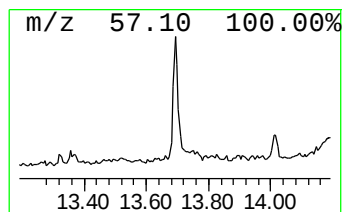
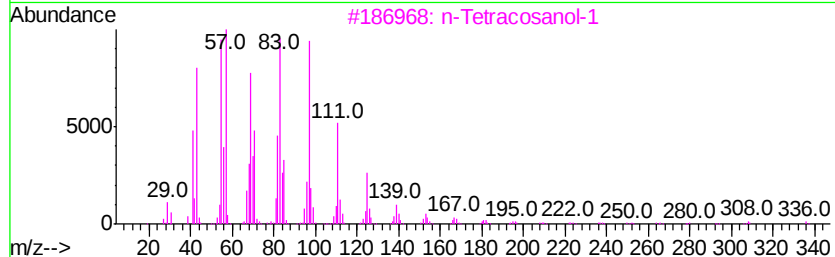
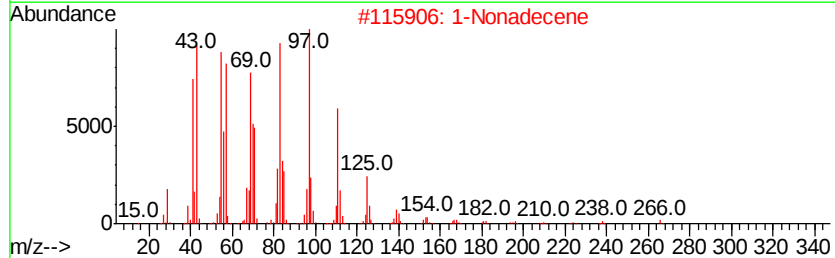
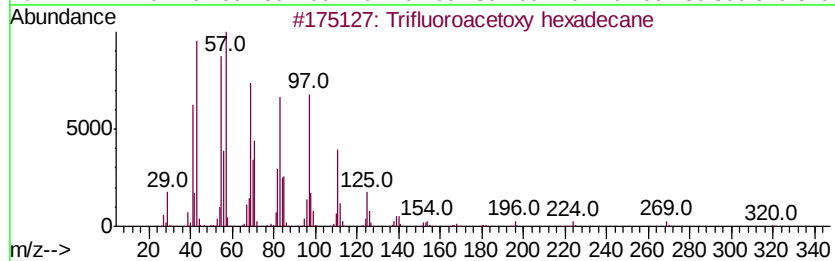
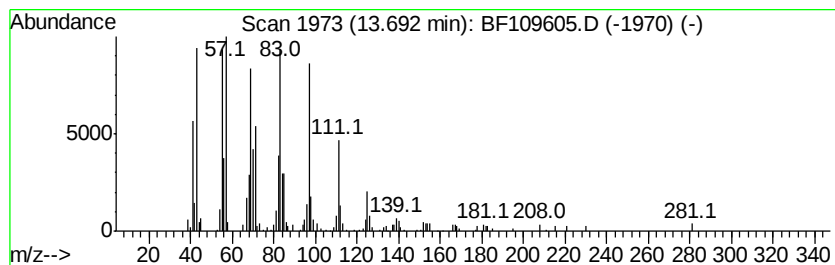
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	7.38 ng	201543	Chrysene-d12	13.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2		1-Nonadecene	266	C19H38	018435-45-5	94
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4		1-Heneicosanol	312	C21H44O	015594-90-8	93
5		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93



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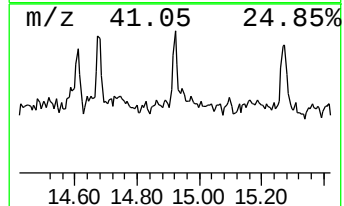
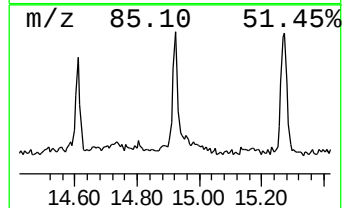
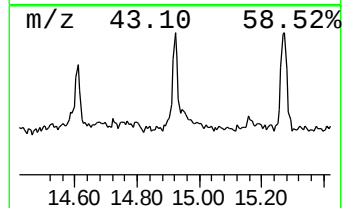
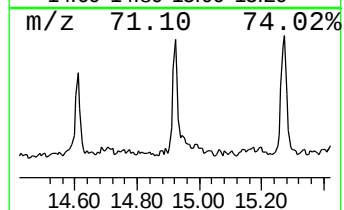
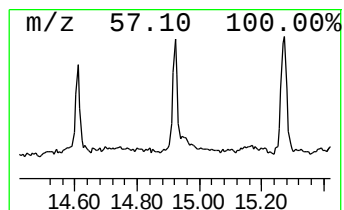
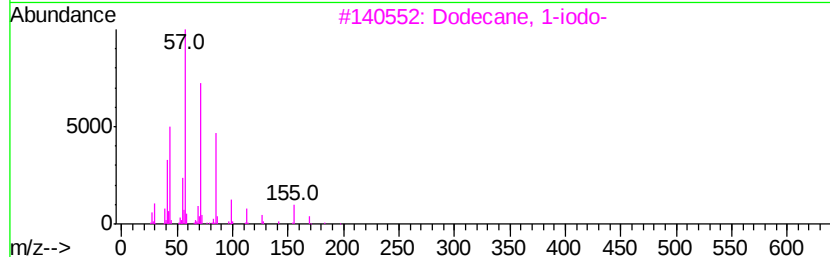
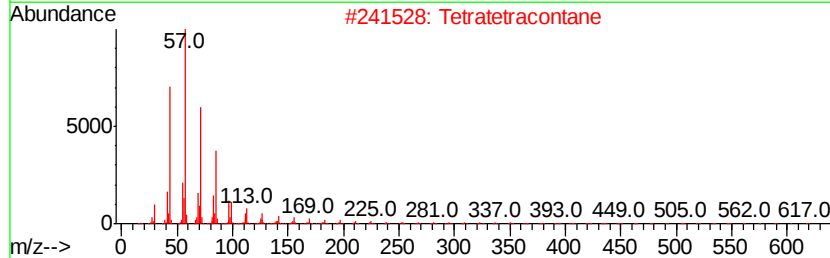
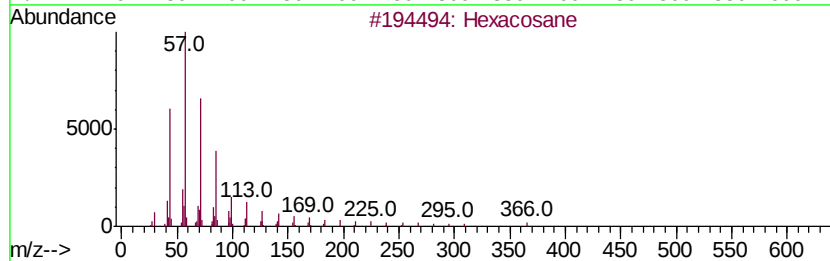
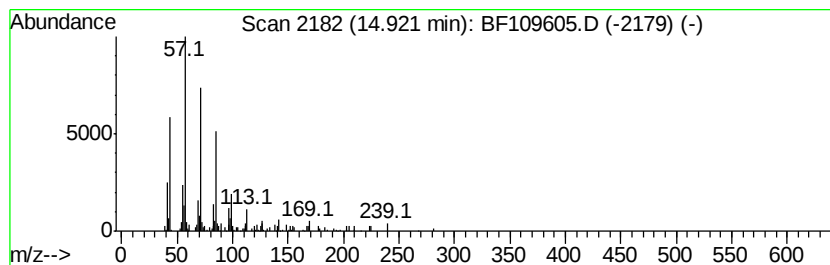
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	3.01 ng	80698	Perylene-d12	15.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Tetratetracontane	619	C44H90	007098-22-8	90
3		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
4		Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	86
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100418\
Data File : BF109605.D
Acq On : 4 Oct 2018 23:22
Operator : JU/SJ
Sample : J5237-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BSS-GW1

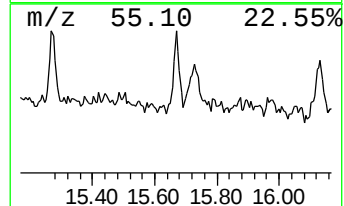
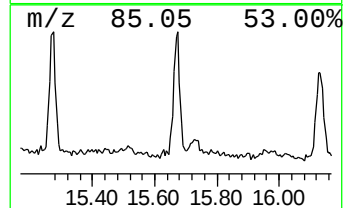
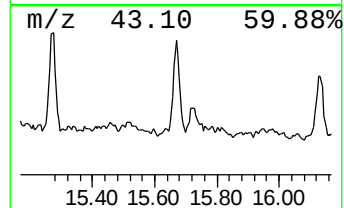
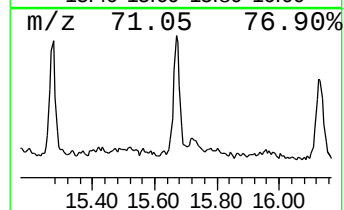
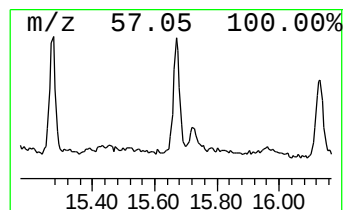
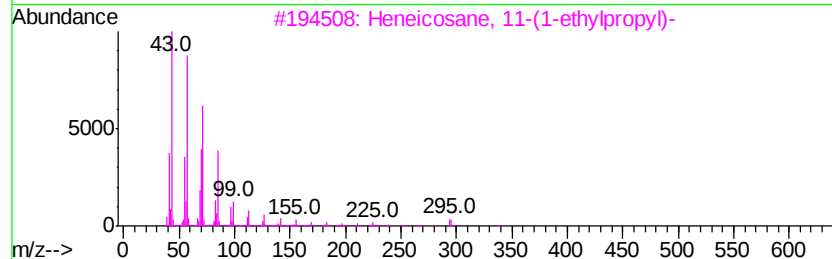
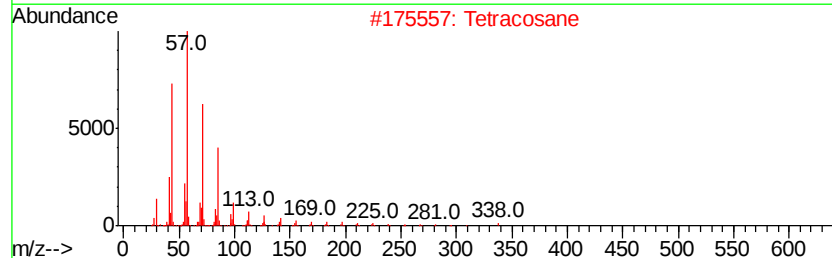
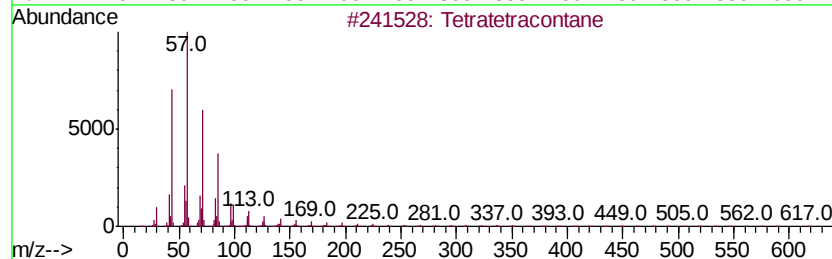
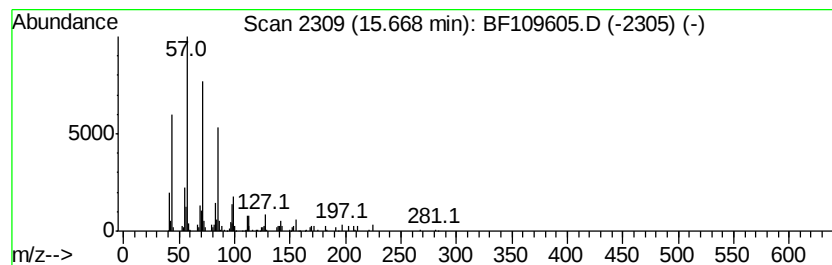
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetratetracontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	3.61 ng	96930	Perylene-d12	15.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	91
2		Tetracosane	338	C24H50	000646-31-1	91
3		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5		triacontane	422	C30H62	000638-68-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100418\
Data File : BF109605.D
Acq On : 4 Oct 2018 23:22
Operator : JU/SJ
Sample : J5237-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BSS-GW1

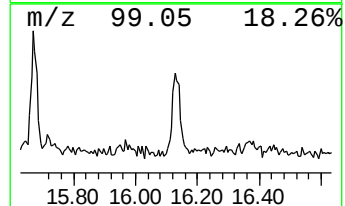
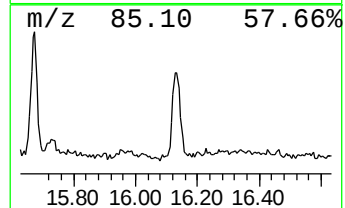
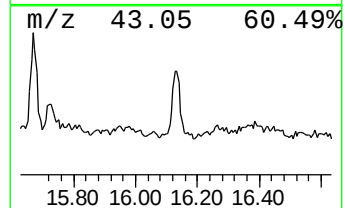
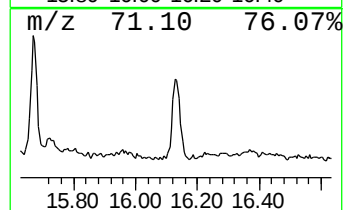
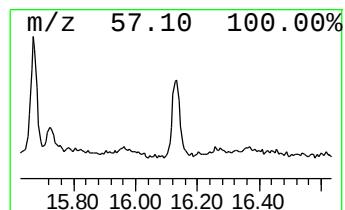
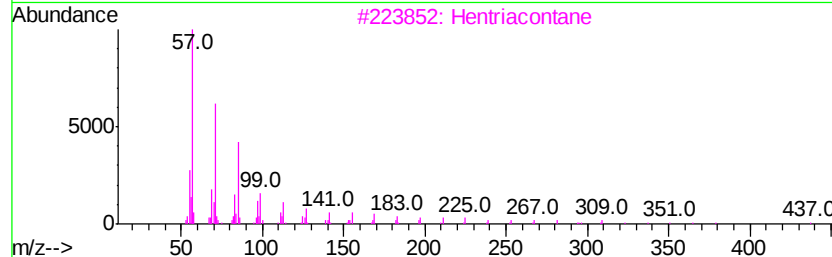
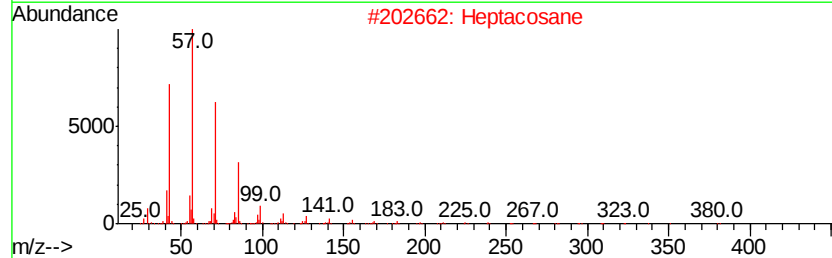
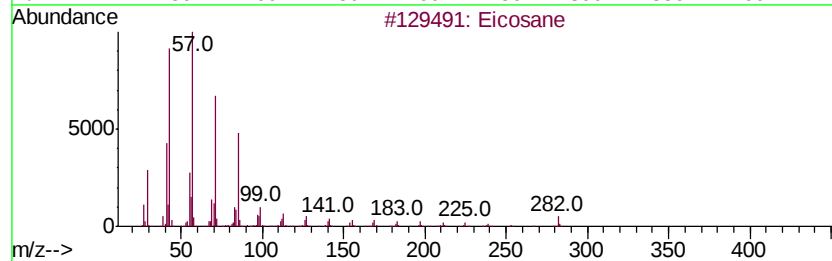
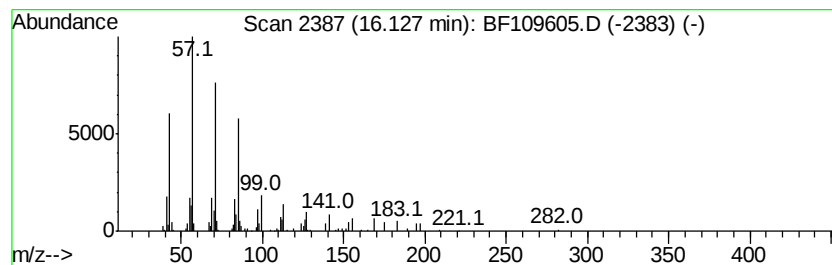
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	2.94 ng	78947	Perylene-d12	15.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	93
2		Heptacosane	380	C27H56	000593-49-7	91
3		Hentriacontane	437	C31H64	000630-04-6	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Octadecane	254	C18H38	000593-45-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100418\
Data File : BF109605.D
Acq On : 4 Oct 2018 23:22
Operator : JU/SJ
Sample : J5237-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BSS-GW1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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...	4.89	2.2	ng	51913	1	6.70	478866	20.0
unknown6.48	6.48	67.3	ng	1612660	1	6.70	478866	20.0
n-Hexadecanoic acid	11.75	7.0	ng	177576	4	11.21	506012	20.0
Octadecanoic acid	12.53	2.8	ng	77449	5	13.84	546015	20.0
Trifluoroacetoxy ...	13.69	7.4	ng	201543	5	13.84	546015	20.0
Hexacosane	14.92	3.0	ng	80698	6	15.24	536947	20.0
Tetratetracontane	15.67	3.6	ng	96930	6	15.24	536947	20.0
Eicosane	16.13	2.9	ng	78947	6	15.24	536947	20.0