

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF111017\
 Data File : BF100415.D
 Acq On : 11 Nov 2017 2:34
 Operator : SJ/JU
 Sample : I6355-05
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 110317-TIFR-F-D-B

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:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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	2.210	17	21	36	rVB	79220	142973	3.33%	0.528%
2	5.122	513	516	525	rVB	307444	337301	7.85%	1.246%
3	5.516	579	583	587	rBV	1905458	1741705	40.53%	6.436%
4	6.516	749	753	756	rBV	1317411	1167105	27.16%	4.313%
5	6.545	756	758	763	rVB	67570	55458	1.29%	0.205%
6	6.669	774	779	782	rBV	2907144	2610421	60.75%	9.646%
7	6.904	815	819	822	rVB	958854	884171	20.58%	3.267%
8	7.063	841	846	849	rBV	3081681	3091186	71.94%	11.422%
9	7.469	909	915	918	rBV	2538847	2699709	62.83%	9.976%
10	8.180	1032	1036	1040	rBV	1216588	1072425	24.96%	3.963%
11	9.263	1214	1220	1223	rBV	4173271	4296900	100.00%	15.878%
12	9.645	1282	1285	1289	rBV	66688	59129	1.38%	0.218%
13	9.939	1329	1335	1343	rVB	1169114	1061416	24.70%	3.922%
14	10.604	1445	1448	1452	rBV	79102	63109	1.47%	0.233%
15	10.727	1464	1469	1472	rBV	1534108	1477244	34.38%	5.459%
16	11.421	1584	1587	1591	rBV	963359	863908	20.11%	3.192%
17	12.821	1822	1825	1828	rBV	140190	117721	2.74%	0.435%
18	12.880	1831	1835	1836	rVV2	40235	51153	1.19%	0.189%
19	12.898	1836	1838	1844	rVB	47820	49158	1.14%	0.182%
20	13.010	1853	1857	1860	rBV	3445997	3335351	77.62%	12.325%
21	13.527	1942	1945	1949	rVB	109387	90753	2.11%	0.335%
22	13.898	2005	2008	2015	rVB2	34627	44627	1.04%	0.165%
23	14.062	2032	2036	2042	rBV	882684	803963	18.71%	2.971%
24	15.545	2283	2288	2298	rBV	467757	651737	15.17%	2.408%
25	16.009	2364	2367	2373	rVB2	40889	55781	1.30%	0.206%
26	16.527	2451	2455	2465	rVB2	49048	92265	2.15%	0.341%
27	17.133	2553	2558	2566	rVB3	35365	78655	1.83%	0.291%
28	17.862	2676	2682	2691	rVB5	27894	67184	1.56%	0.248%

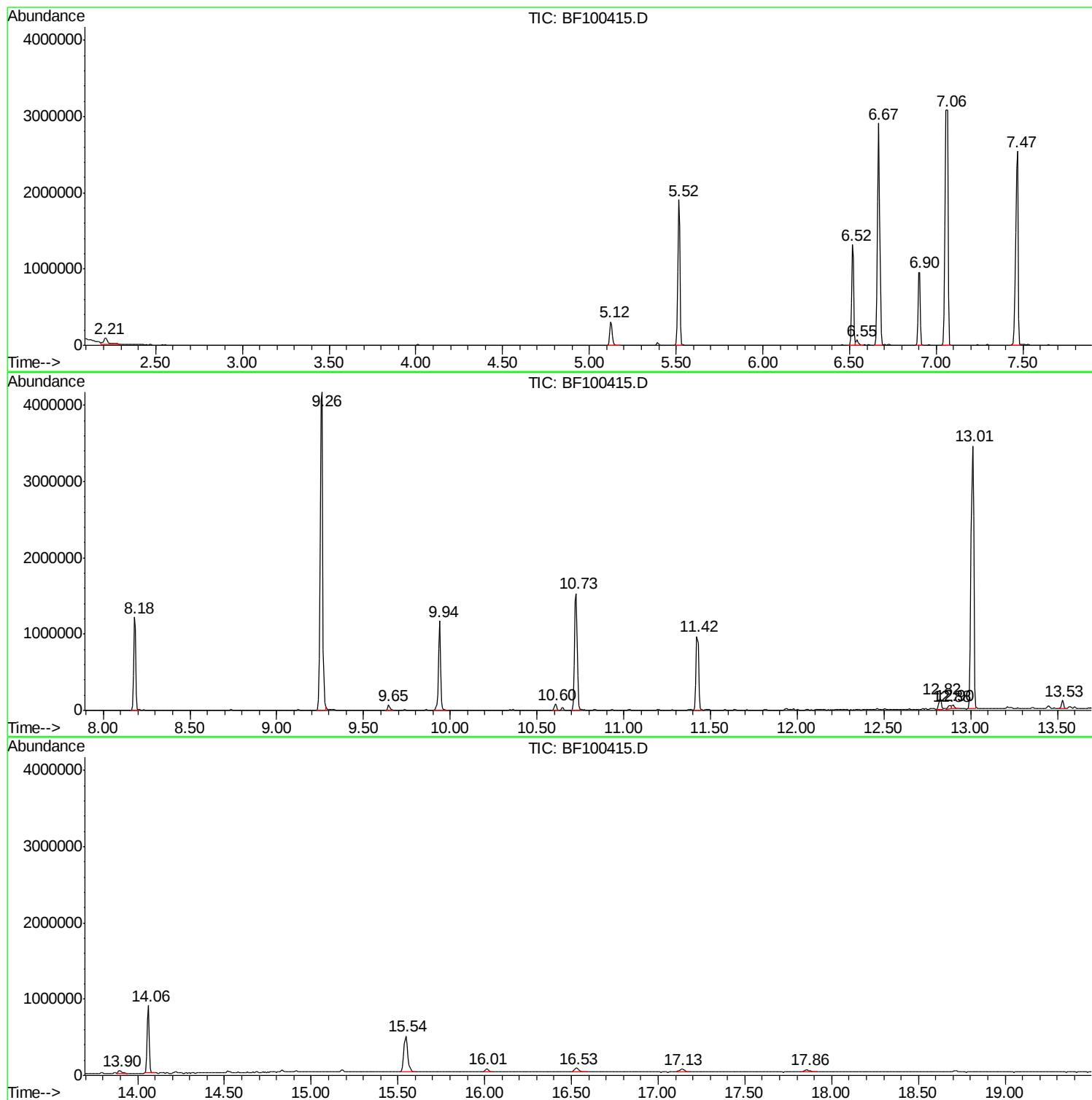
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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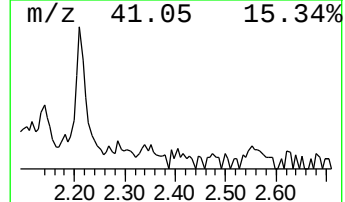
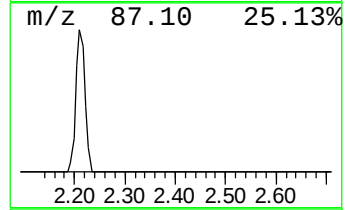
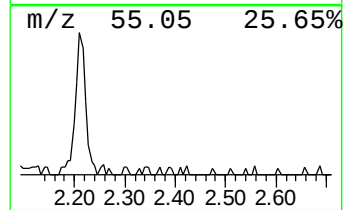
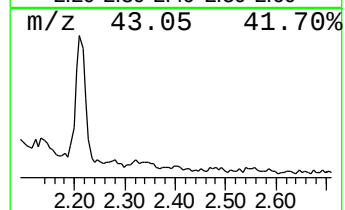
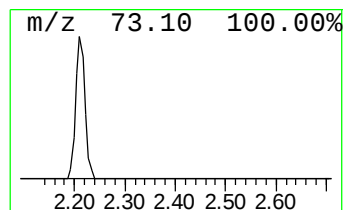
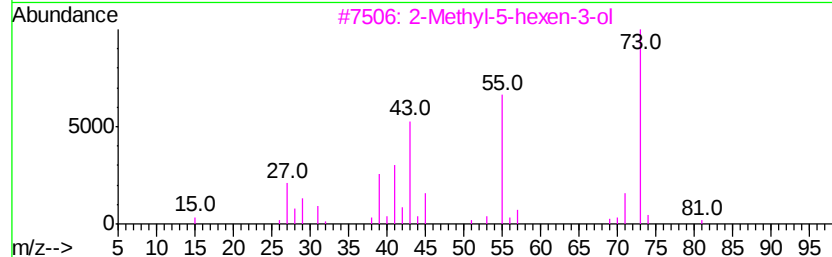
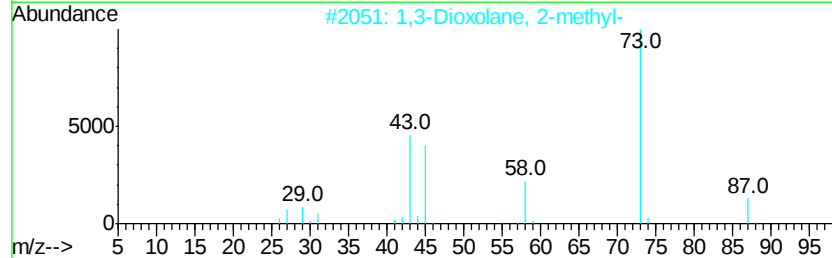
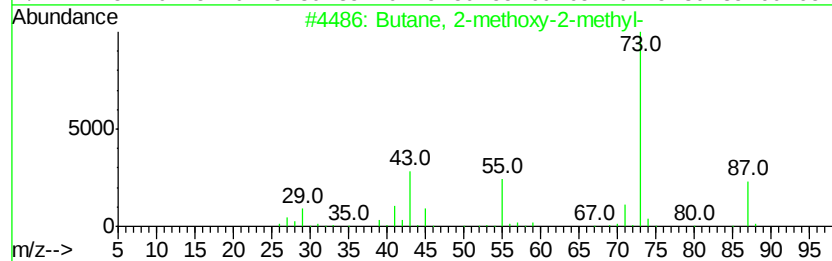
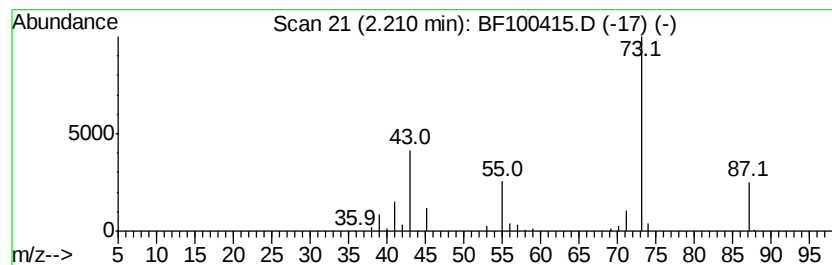
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.21	3.23 ng	142973	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	16
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9



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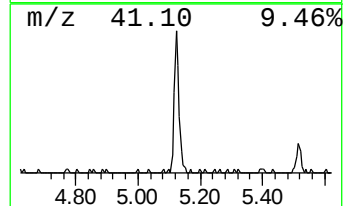
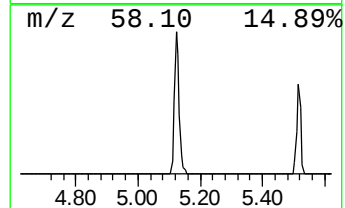
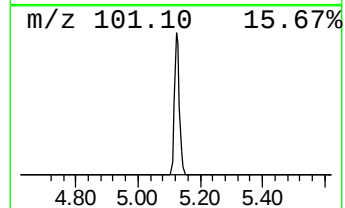
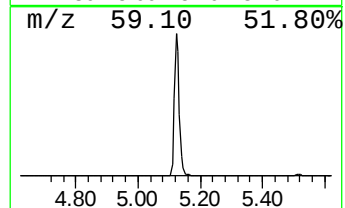
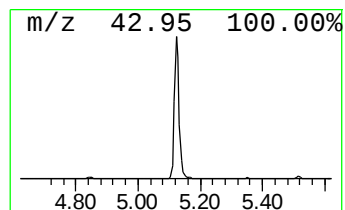
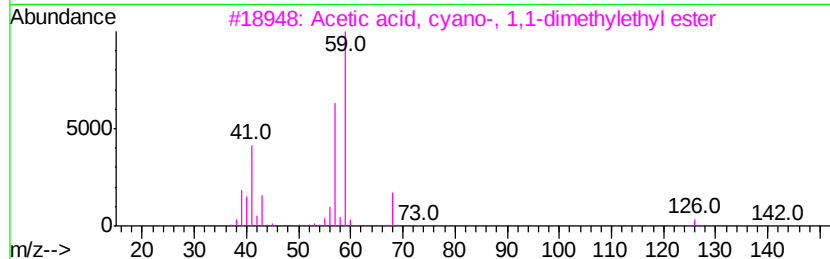
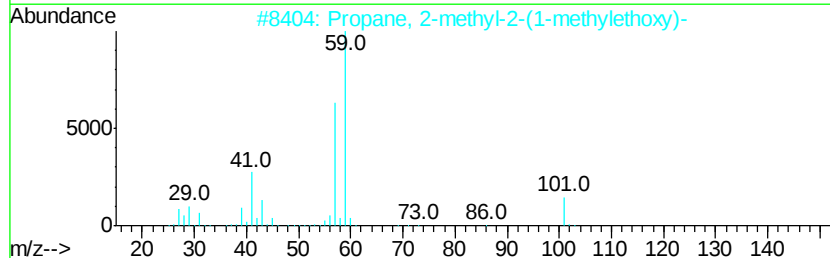
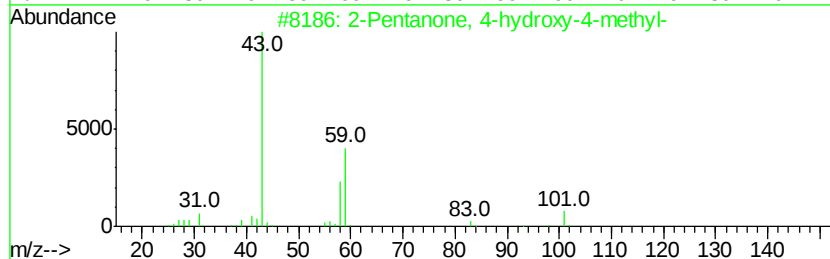
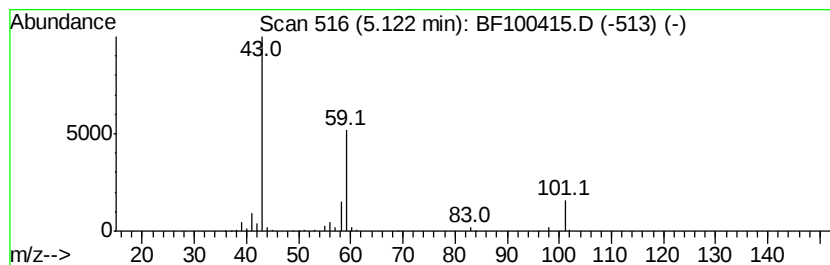
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	7.63 ng	337301	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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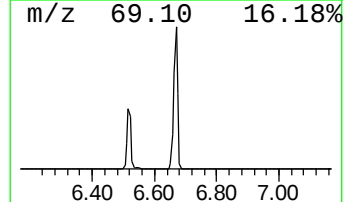
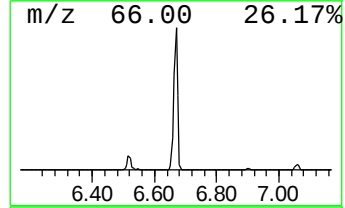
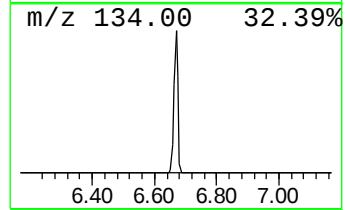
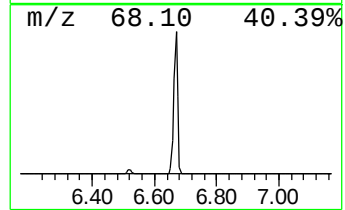
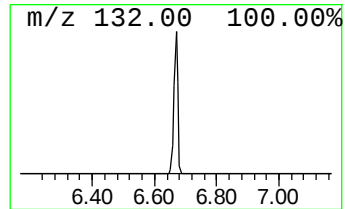
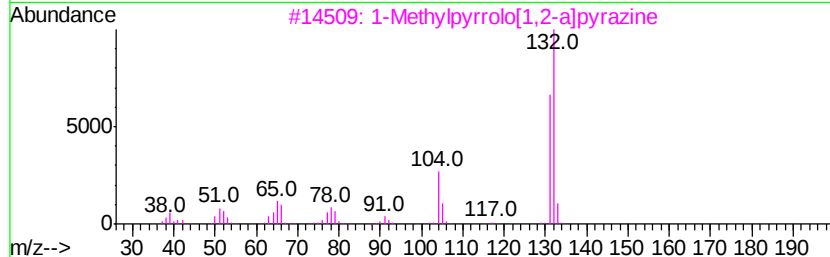
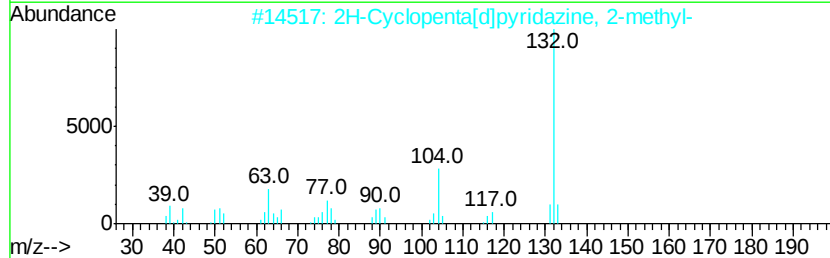
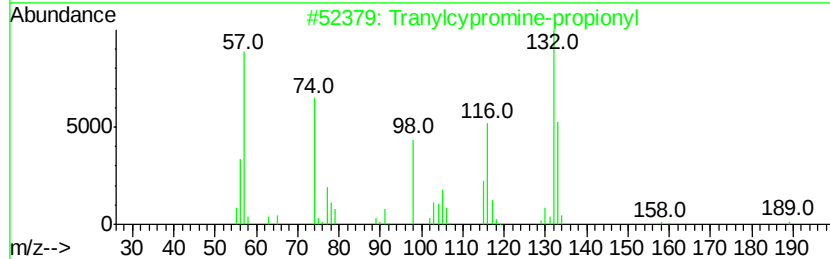
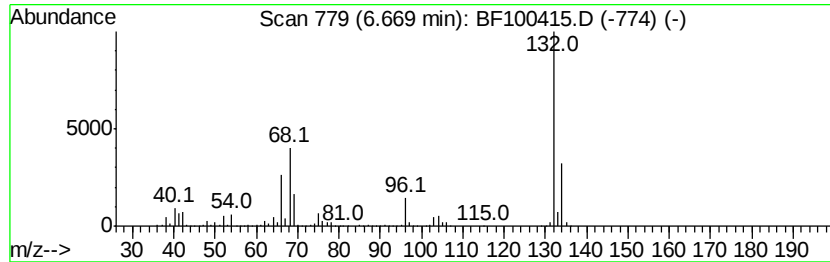
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Peak Number 3 unknown6.67 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	59.05 ng	2610420	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
2		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
3		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Aminoindole	132	C8H8N2	005192-03-0	9



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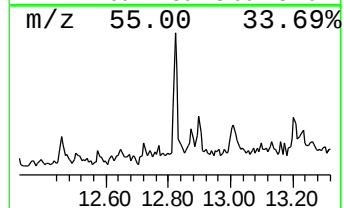
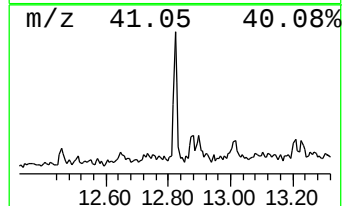
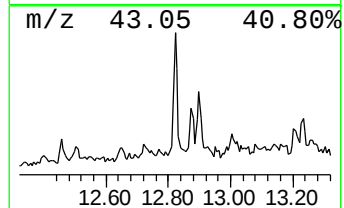
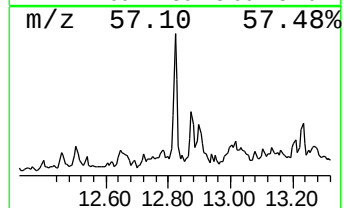
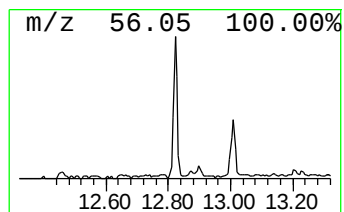
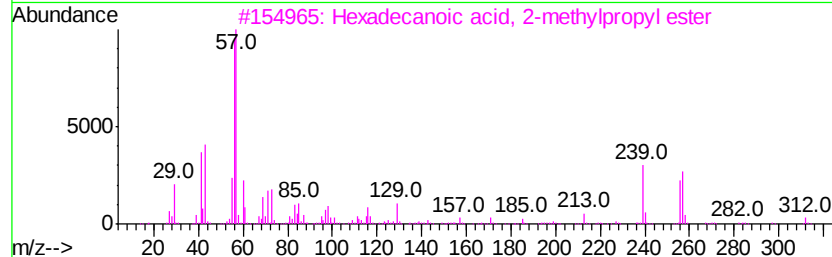
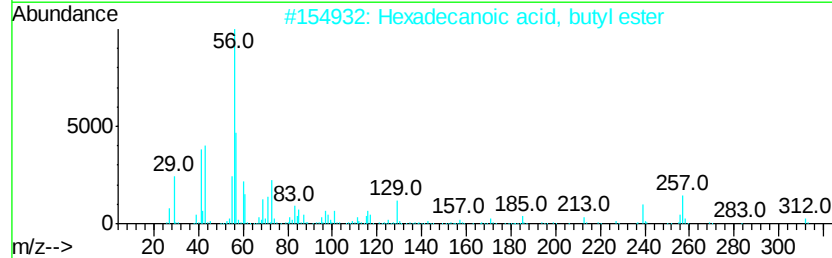
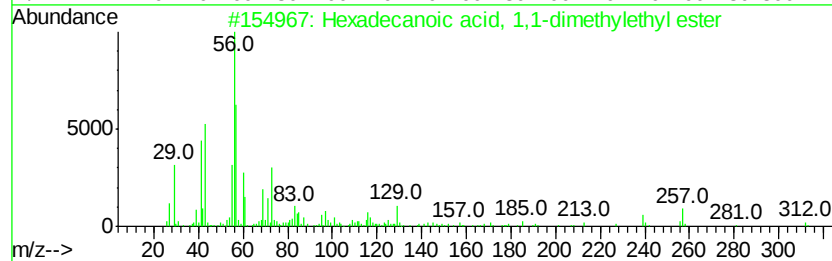
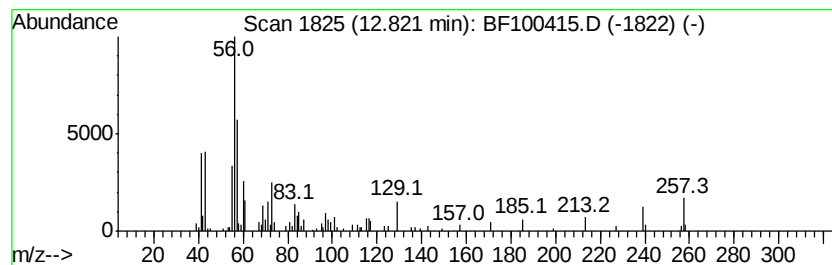
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Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.82	2.93 ng	117721	Chrysene-d12	14.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	43
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38
5		Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	38



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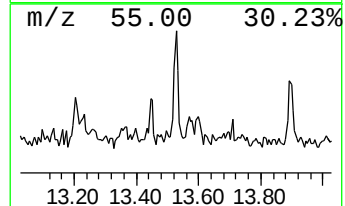
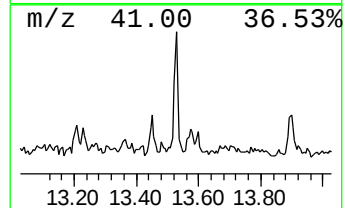
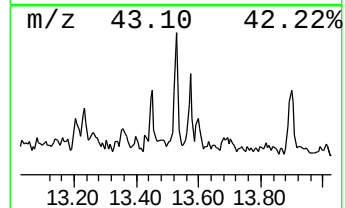
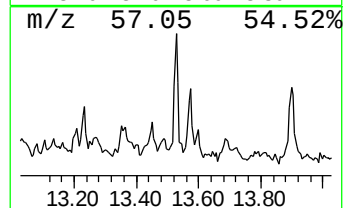
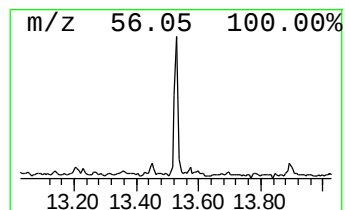
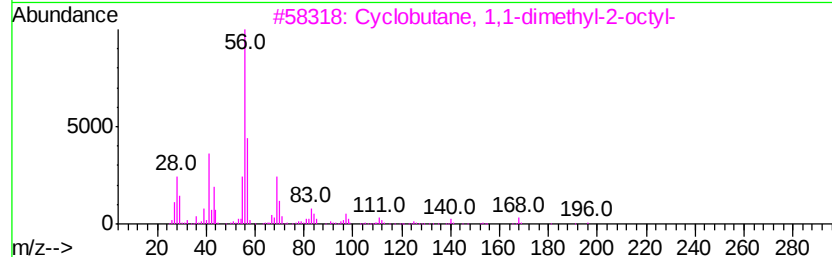
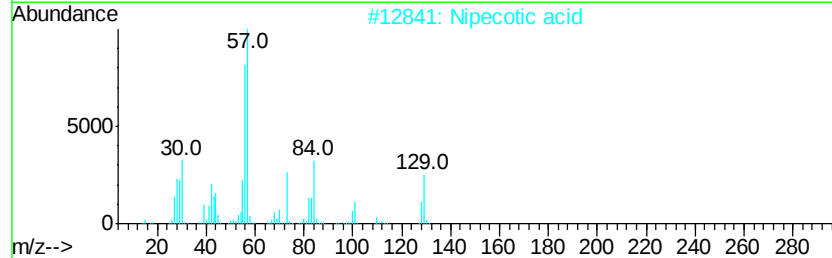
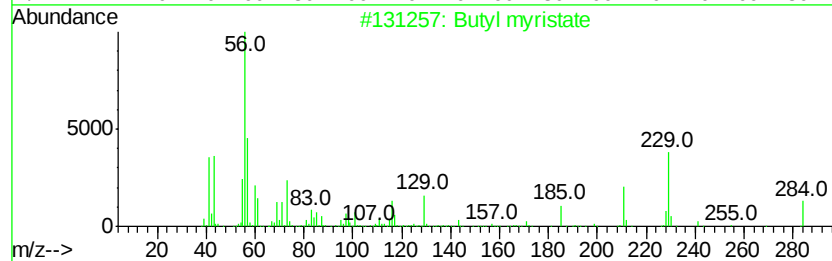
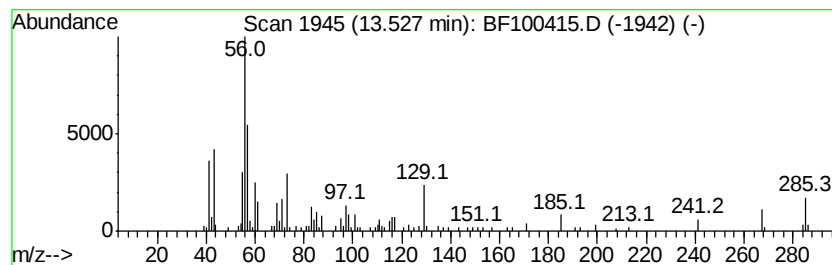
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Peak Number 6 unknown13.53 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	2.26 ng	90753	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butyl myristate	284	C18H36O2	000110-36-1	45
2		Nipecotic acid	129	C6H11NO2	000498-95-3	38
3		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
4		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	38
5		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35



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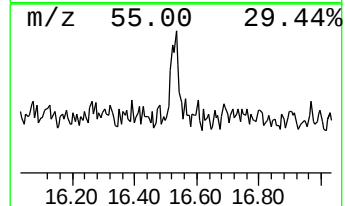
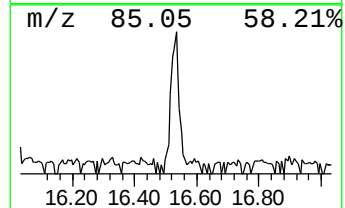
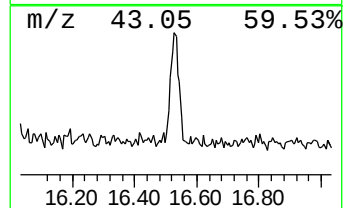
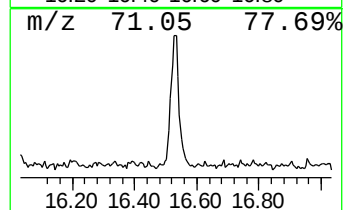
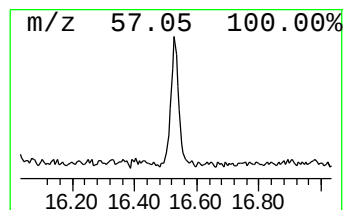
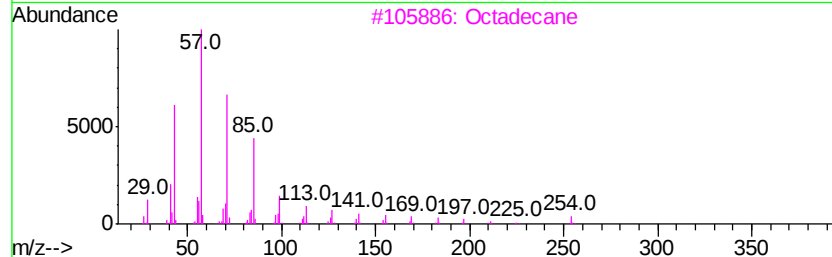
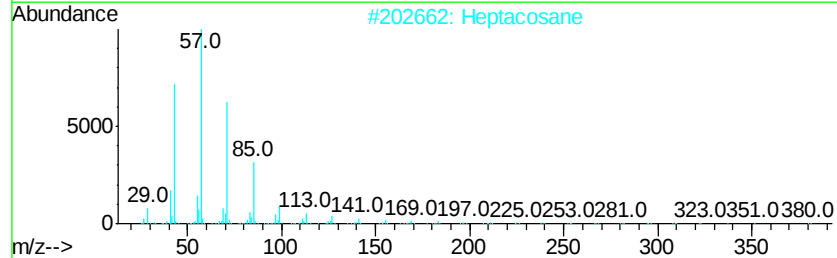
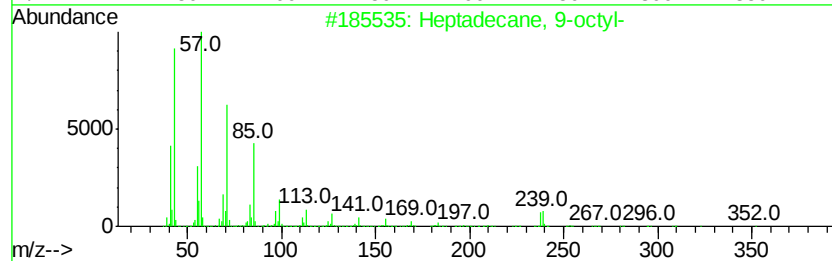
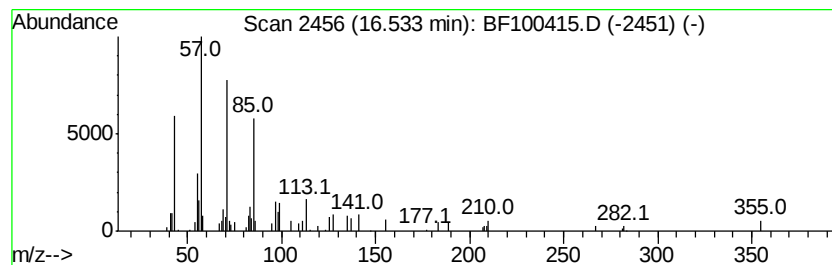
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane, 9-octyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	2.83 ng	92265	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
2		Heptacosane	380	C27H56	000593-49-7	86
3		Octadecane	254	C18H38	000593-45-3	86
4		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86
5		Pentacosane	352	C25H52	000629-99-2	83



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF111017\
Data File : BF100415.D
Acq On : 11 Nov 2017 2:34
Operator : SJ/JU
Sample : I6355-05
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
110317-TIFR-F-D-B

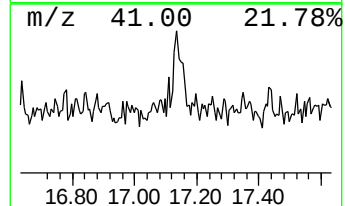
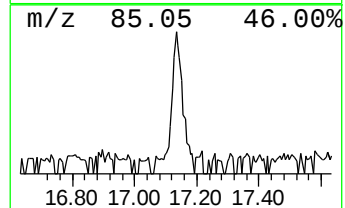
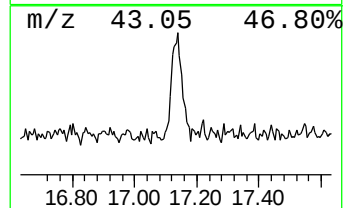
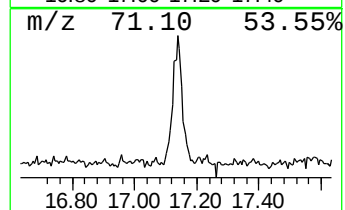
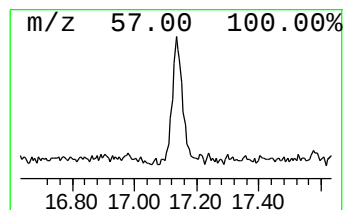
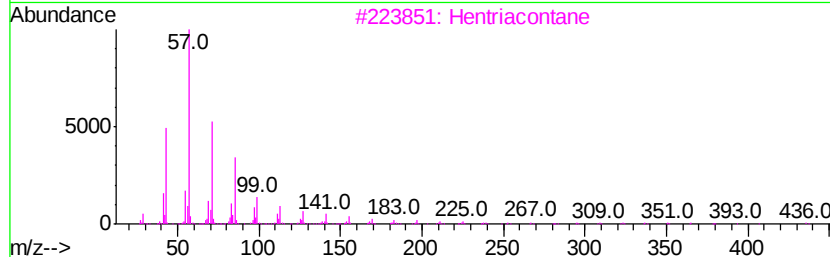
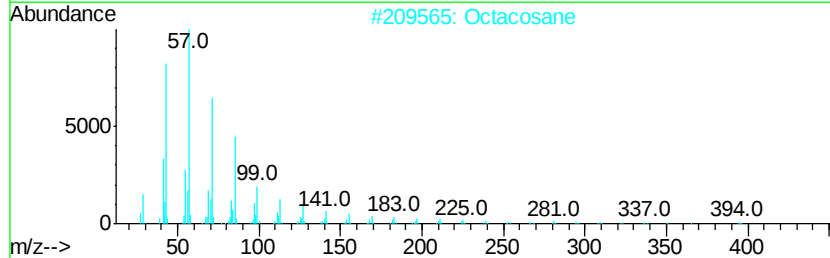
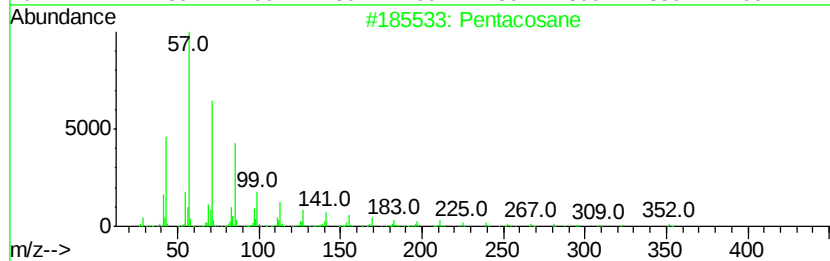
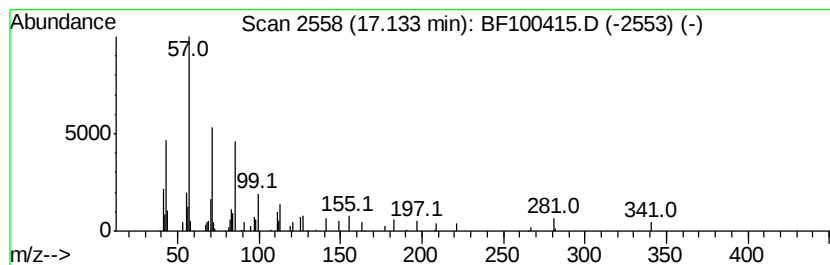
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.13	2.41 ng	78655	Perylene-d12	15.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane		352	C25H52	000629-99-2	87
2	Octacosane		394	C28H58	000630-02-4	87
3	Hentriacontane		437	C31H64	000630-04-6	86
4	Eicosane		282	C20H42	000112-95-8	86
5	Heneicosane		296	C21H44	000629-94-7	83



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF111017\
Data File : BF100415.D
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Operator : SJ/JU
Sample : I6355-05
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
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ClientSampleId :
110317-TIFR-F-D-B

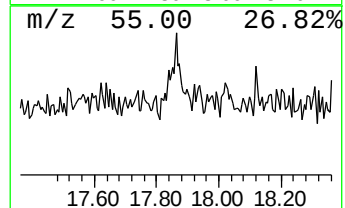
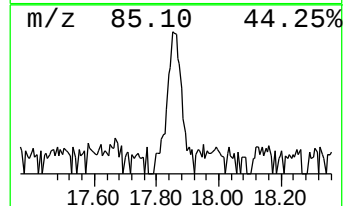
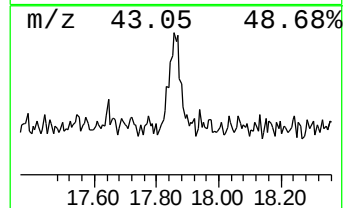
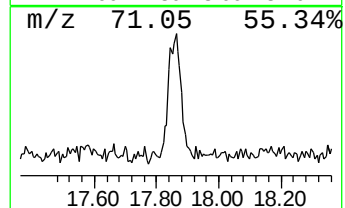
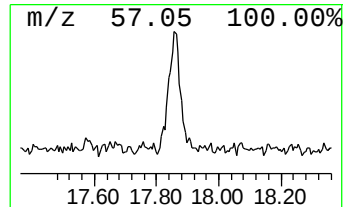
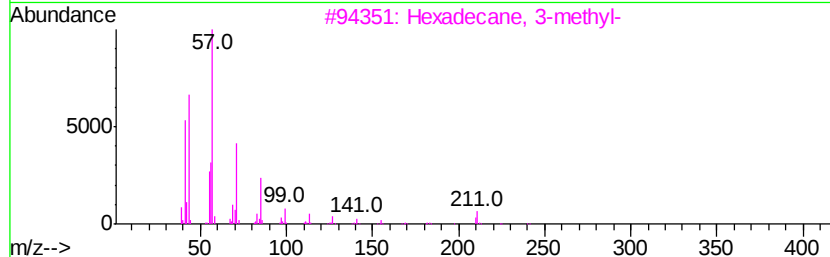
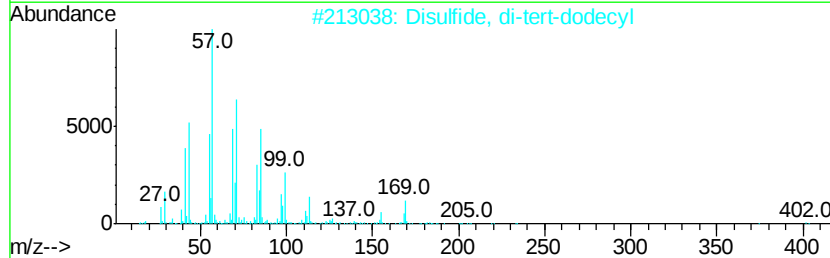
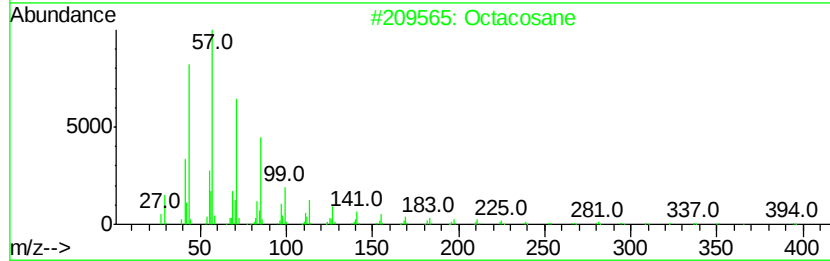
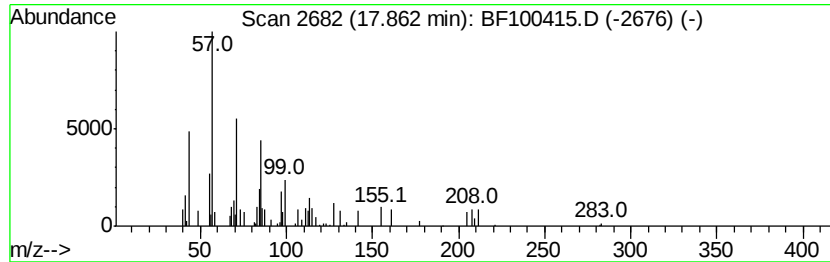
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.86	2.06 ng	67184	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	80
2		Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	78
3		Hexadecane, 3-methyl-	240	C17H36	006418-43-5	64
4		Hentriacontane	437	C31H64	000630-04-6	64
5		Tetrapentacontane	759	C54H110	005856-66-6	64



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF111017\
Data File : BF100415.D
Acq On : 11 Nov 2017 2:34
Operator : SJ/JU
Sample : I6355-05
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
110317-TIFR-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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
Butane, 2-methoxy...	2.21	3.2	ng	142973	1	6.90	884171	20.0
2-Pentanone, 4-hy...	5.12	7.6	ng	337301	1	6.90	884171	20.0
unknown6.67	6.67	59.0	ng	2610420	1	6.90	884171	20.0
Hexadecanoic acid...	12.82	2.9	ng	117721	5	14.06	803963	20.0
unknown13.53	13.53	2.3	ng	90753	5	14.06	803963	20.0
Heptadecane, 9-oc...	16.53	2.8	ng	92265	6	15.54	651737	20.0
Pentacosane	17.13	2.4	ng	78655	6	15.54	651737	20.0
Octacosane	17.86	2.1	ng	67184	6	15.54	651737	20.0