

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082418\
 Data File : BF108471.D
 Acq On : 24 Aug 2018 18:53
 Operator : JU/SJ
 Sample : J4581-07
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP1-Q3-B3

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-BF080818.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	2.372	3	6	15	rVB	898314	1179405	34.94%	3.839%
2	5.248	491	495	503	rBV	140264	178185	5.28%	0.580%
3	5.630	555	560	563	rBV	3009102	2810726	83.27%	9.150%
4	6.625	723	729	742	rBV	2898918	3090453	91.56%	10.060%
5	6.772	749	754	757	rBV	3204279	3019019	89.44%	9.828%
6	7.001	789	793	796	rBV	832139	772374	22.88%	2.514%
7	7.154	815	819	823	rBV	2372760	2094901	62.06%	6.819%
8	7.560	883	888	891	rBV	1917646	1964530	58.20%	6.395%
9	8.283	1006	1011	1025	rBV	1035924	996512	29.52%	3.244%
10	9.354	1188	1193	1197	rBV	3598111	3375384	100.00%	10.988%
11	9.742	1256	1259	1268	rVB	319391	306759	9.09%	0.999%
12	10.042	1305	1310	1320	rVB2	1272936	1179454	34.94%	3.839%
13	10.836	1440	1445	1454	rBV	2478686	2364788	70.06%	7.698%
14	10.924	1457	1460	1466	rVB	29672	38809	1.15%	0.126%
15	11.536	1560	1564	1567	rBV	1233638	1189588	35.24%	3.872%
16	11.560	1567	1568	1572	rVB	108743	76276	2.26%	0.248%
17	12.042	1647	1650	1653	rBV	70312	72504	2.15%	0.236%
18	12.071	1653	1655	1661	rVB2	30090	39572	1.17%	0.129%
19	12.759	1768	1772	1775	rVB	105832	97518	2.89%	0.317%
20	12.989	1804	1811	1816	rBV	130501	163411	4.84%	0.532%
21	13.124	1829	1834	1837	rBV	3539818	3124257	92.56%	10.170%
22	13.330	1864	1869	1872	rVB2	43068	42770	1.27%	0.139%
23	13.671	1923	1927	1930	rBV2	60112	57327	1.70%	0.187%
24	14.001	1979	1983	1987	rBV2	72772	61441	1.82%	0.200%
25	14.065	1987	1994	2005	rBV2	23237	84776	2.51%	0.276%
26	14.189	2010	2015	2018	rBV	864910	799386	23.68%	2.602%
27	14.318	2031	2037	2044	rBV2	79679	81058	2.40%	0.264%
28	14.624	2086	2089	2094	rVB	80867	76828	2.28%	0.250%
29	14.942	2139	2143	2150	rBV2	150585	208496	6.18%	0.679%
30	15.277	2196	2200	2202	rBV	25336	37482	1.11%	0.122%
31	15.312	2202	2206	2212	rVB2	85488	112652	3.34%	0.367%
32	15.742	2271	2279	2289	rVB	572090	826124	24.47%	2.689%
33	16.195	2351	2356	2362	rVB	70497	119855	3.55%	0.390%
34	16.747	2444	2450	2456	rBV2	42081	76899	2.28%	0.250%

LSC Area Percent Report

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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-BF080818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

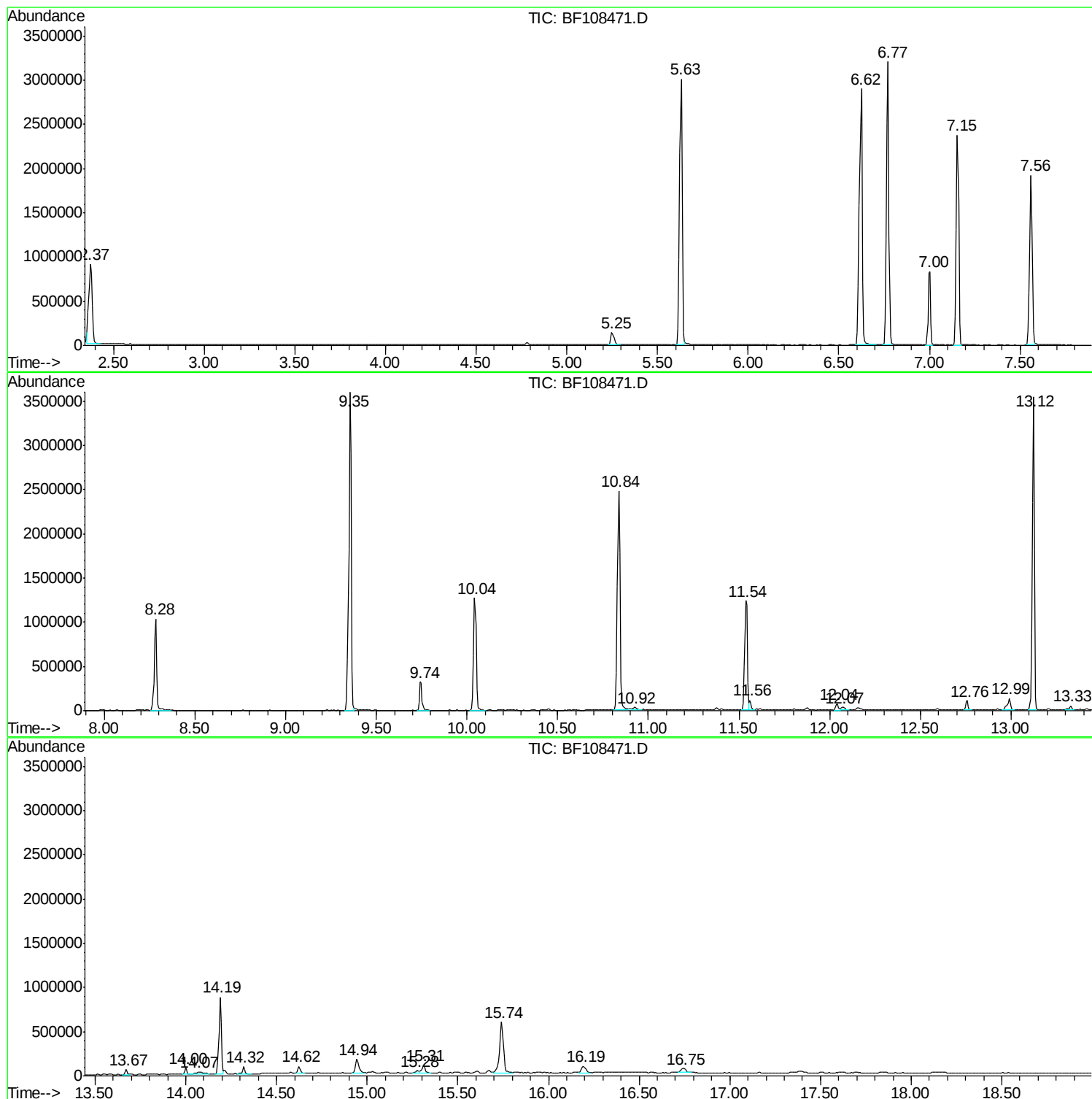
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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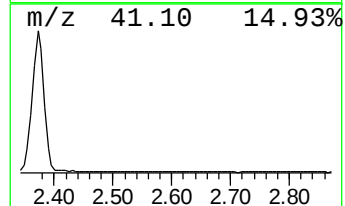
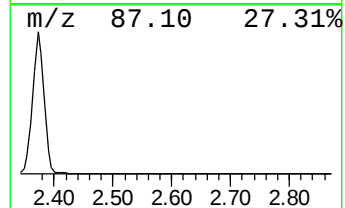
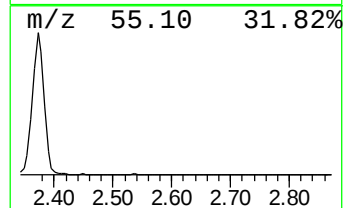
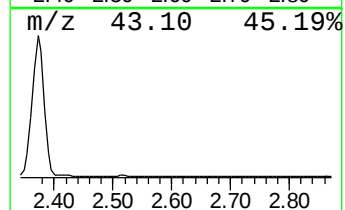
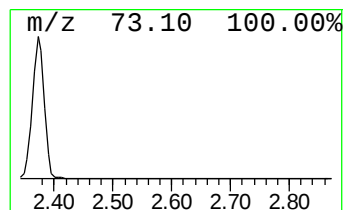
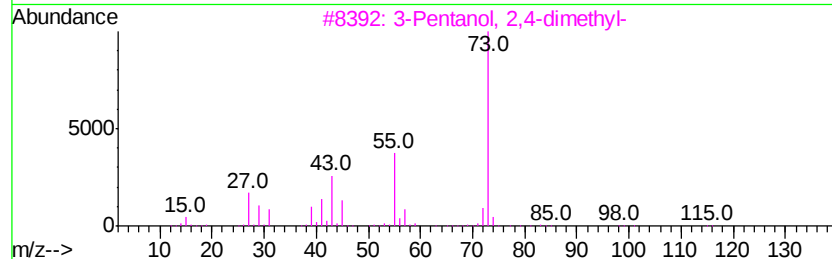
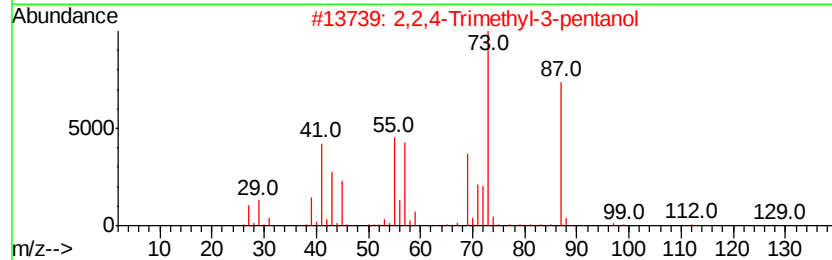
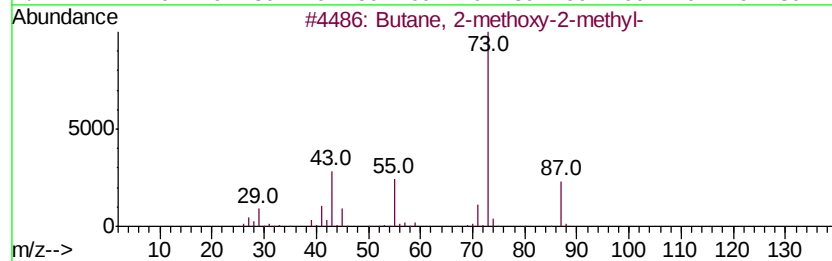
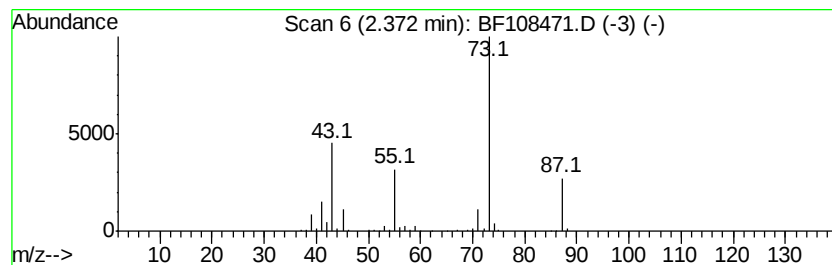
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.37	30.54 ng	1179410	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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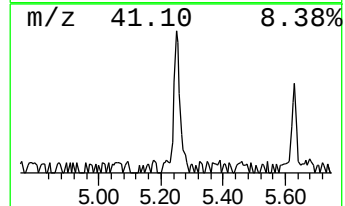
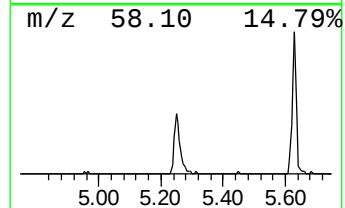
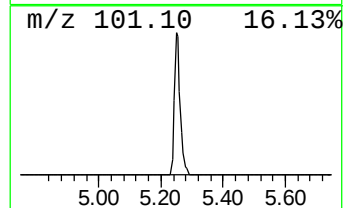
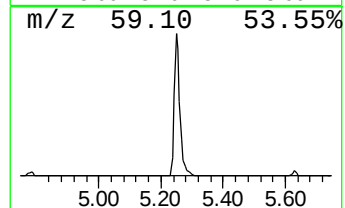
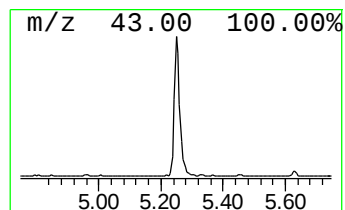
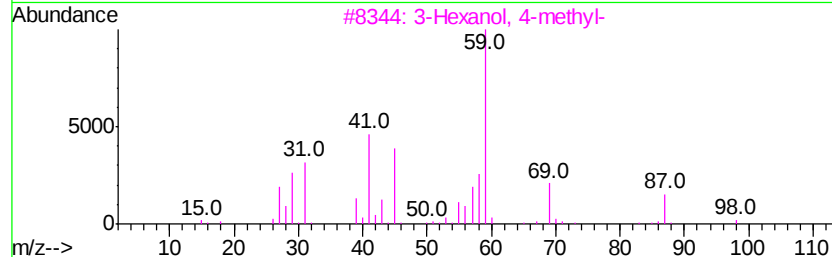
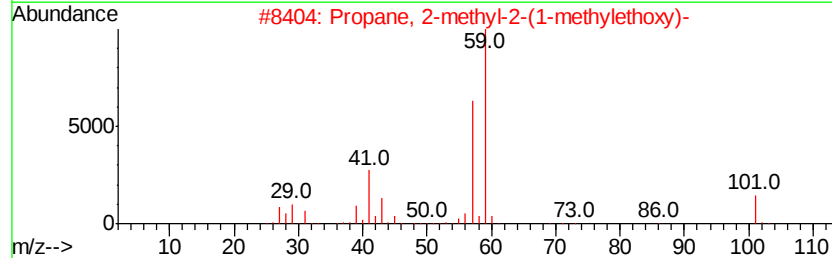
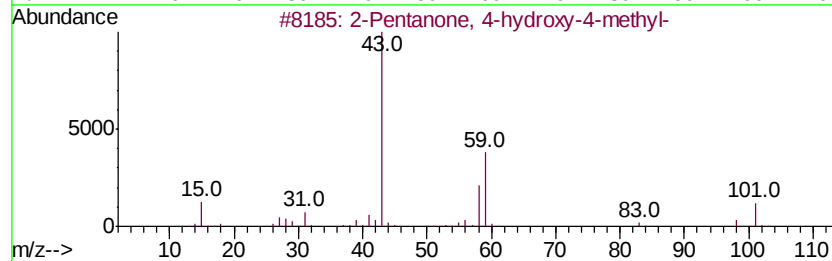
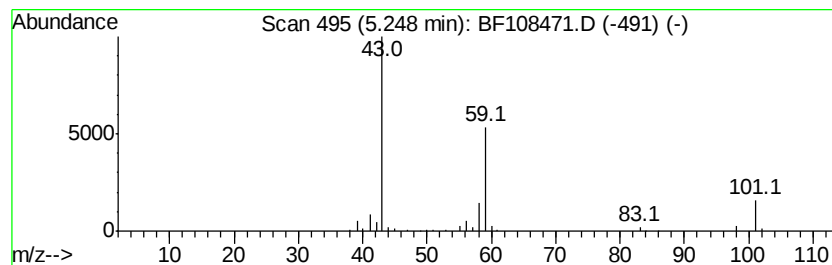
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.25	4.61 ng	178185	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	36
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	25



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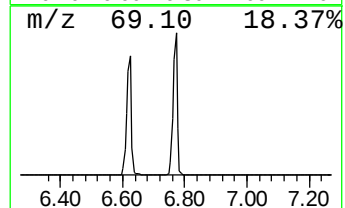
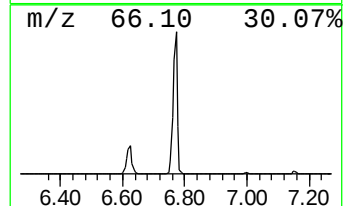
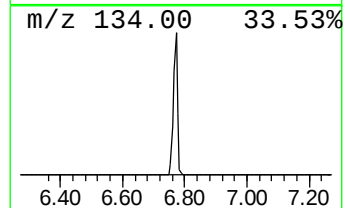
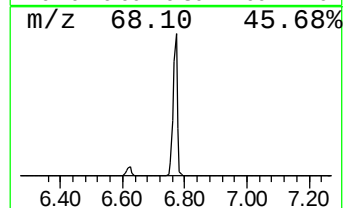
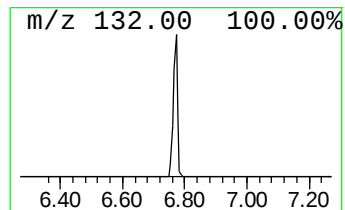
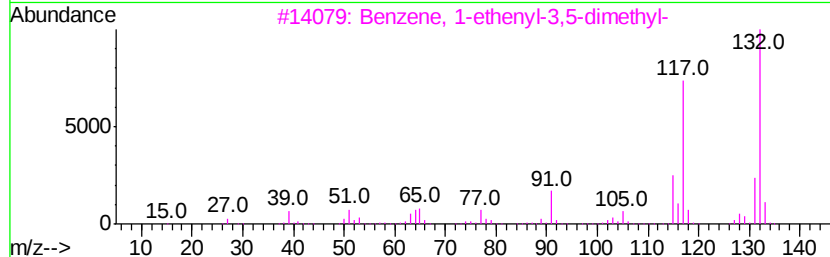
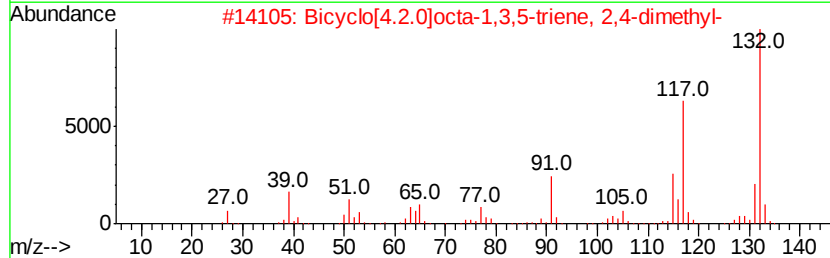
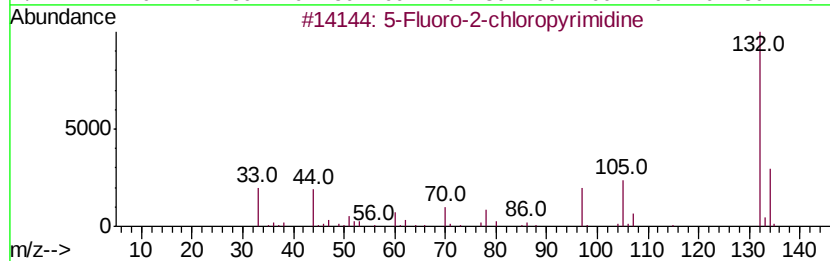
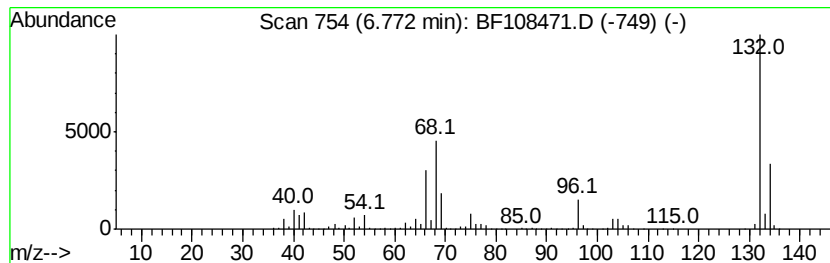
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	78.18 ng	3019020	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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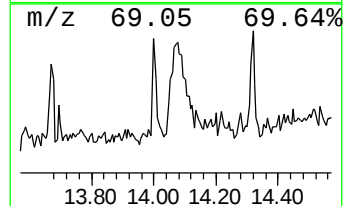
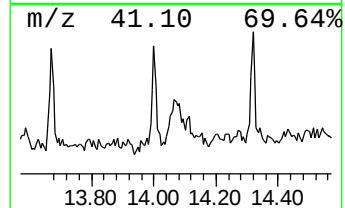
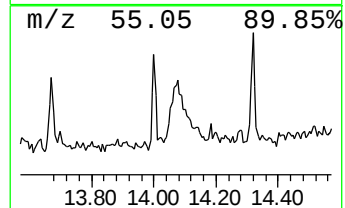
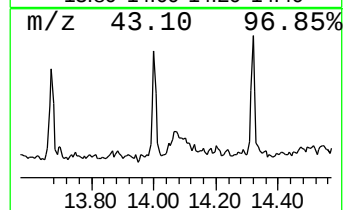
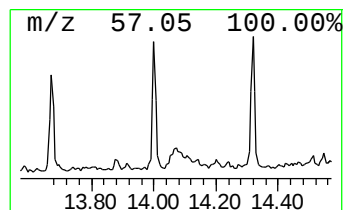
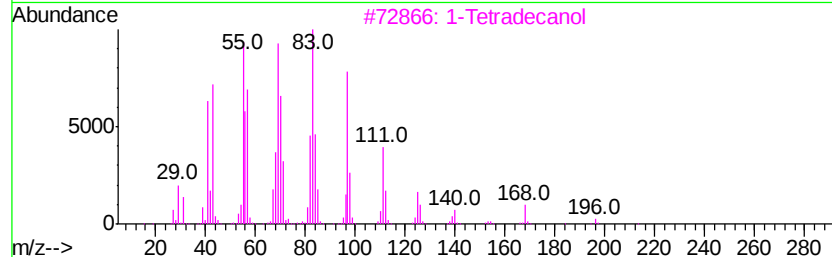
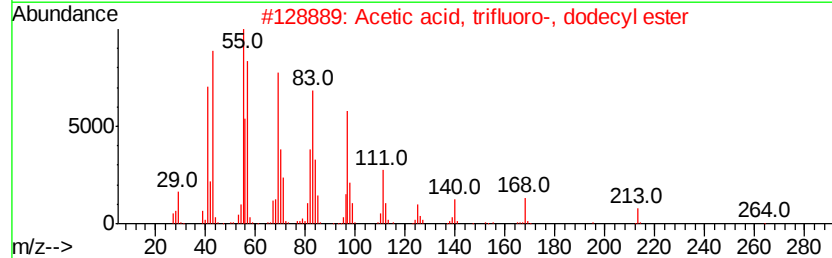
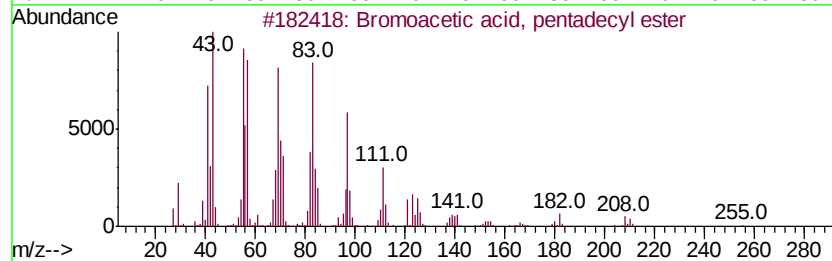
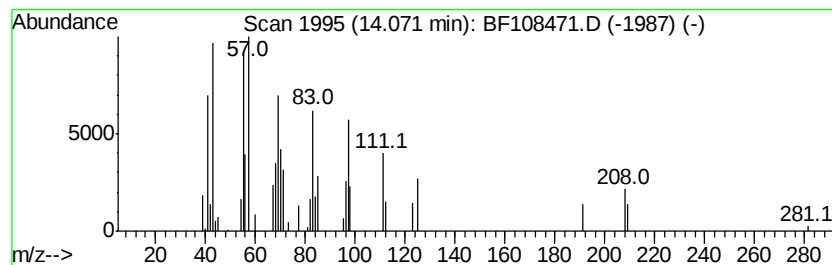
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Bromoacetic acid, pentadecyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.07	2.12 ng	84776	Chrysene-d12	14.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	81
2		Acetic acid, trifluoro-, dodecyl...	282	C14H25F3O2	006222-00-0	81
3		1-Tetradecanol	214	C14H30O	000112-72-1	74
4		n-Tridecan-1-ol	200	C13H28O	000112-70-9	74
5		1-Octadecanol	270	C18H38O	000112-92-5	74



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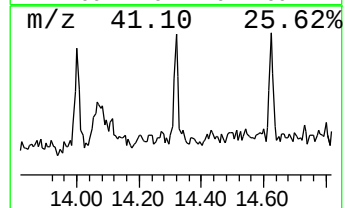
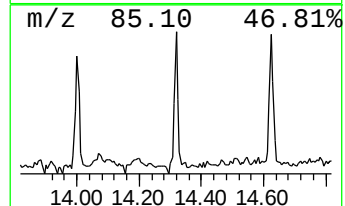
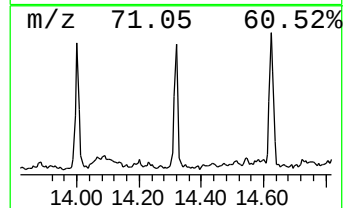
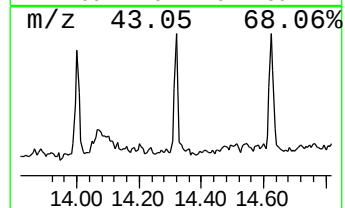
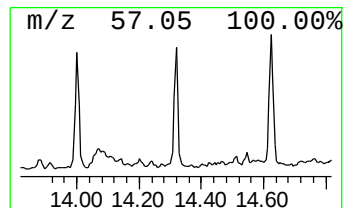
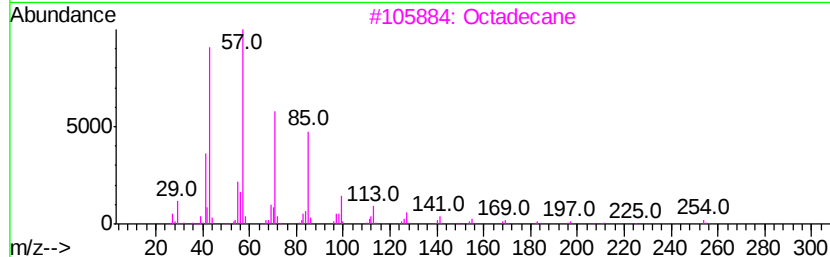
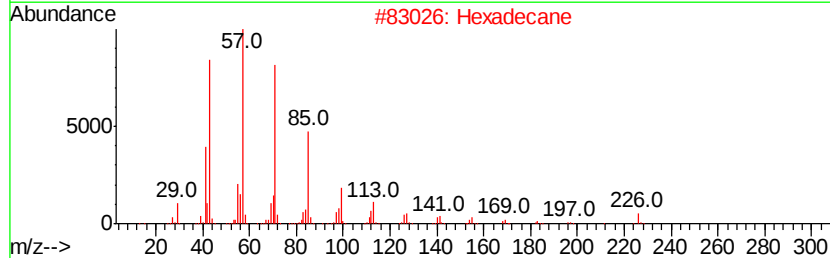
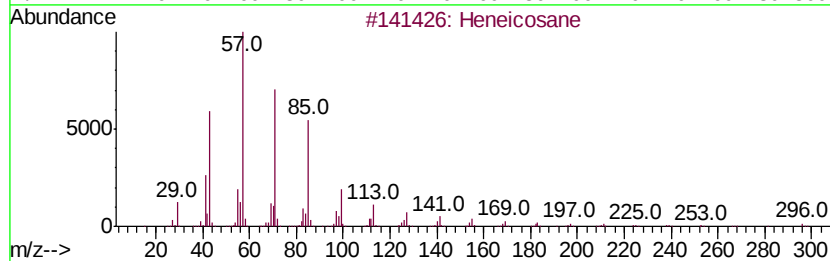
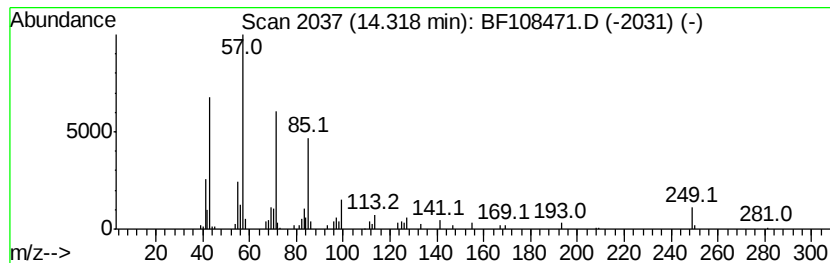
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	2.03 ng	81058	Chrysene-d12	14.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	87
2	Hexadecane		226	C16H34	000544-76-3	83
3	Octadecane		254	C18H38	000593-45-3	83
4	Pentadecane		212	C15H32	000629-62-9	83
5	Nonadecane		268	C19H40	000629-92-5	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082418\
Data File : BF108471.D
Acq On : 24 Aug 2018 18:53
Operator : JU/SJ
Sample : J4581-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q3-B3

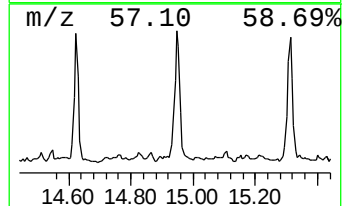
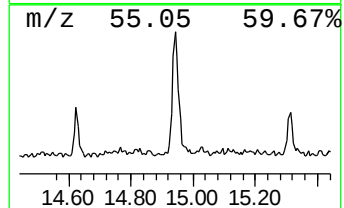
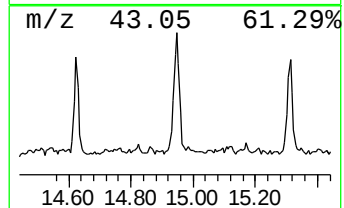
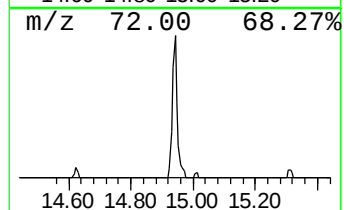
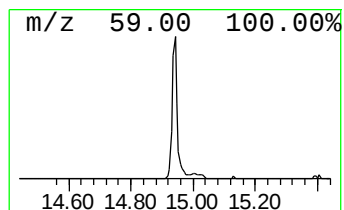
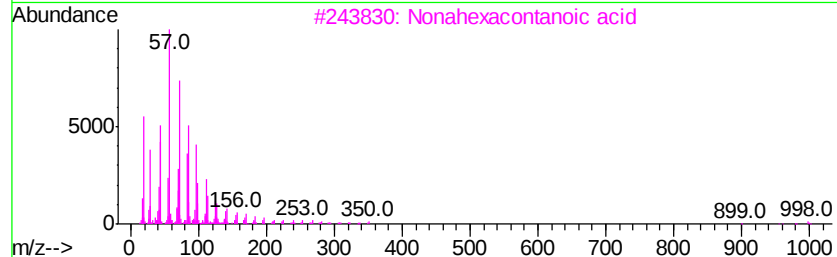
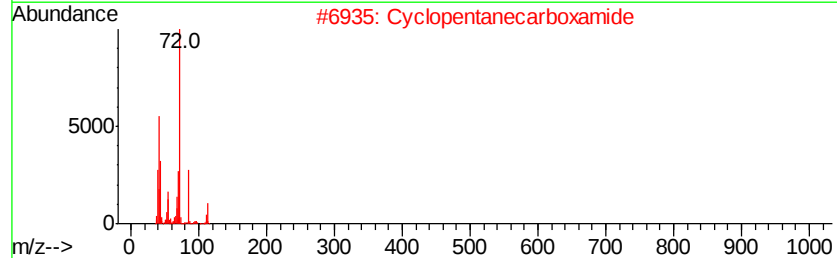
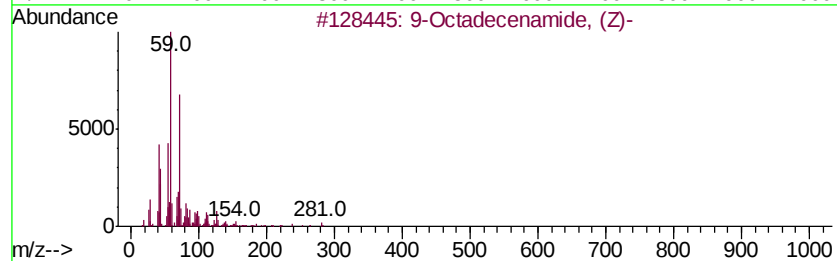
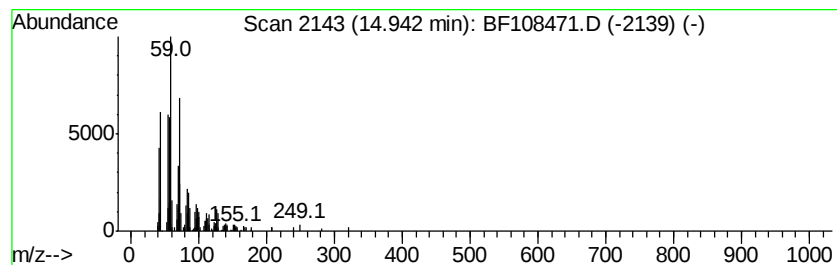
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	5.22 ng	208496	Chrysene-d12	14.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
2		Cyclopentanecarboxamide	113	C6H11NO	003217-94-5	18
3		Nonahexacontanoic acid	999	C69H138O2	040710-32-5	11
4		2-Butene, 1-butoxy-, (E)-	128	C8H16O	056052-72-3	11
5		Cyclopentylsilane	100	C5H12Si	080249-74-7	11



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Operator : JU/SJ
Sample : J4581-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q3-B3

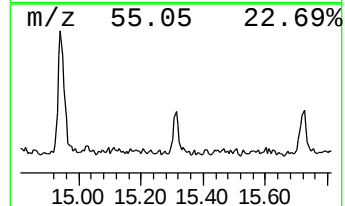
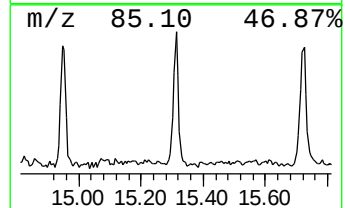
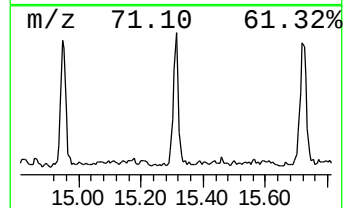
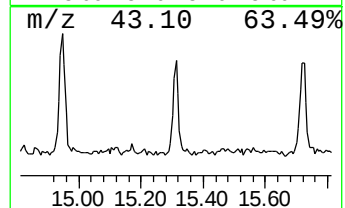
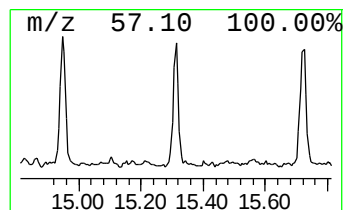
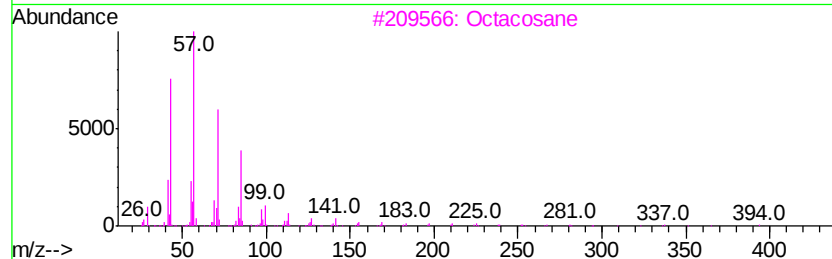
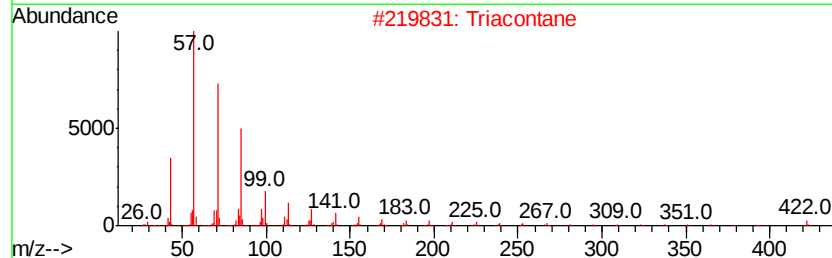
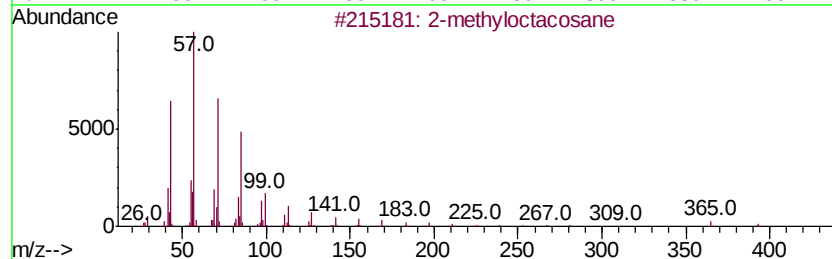
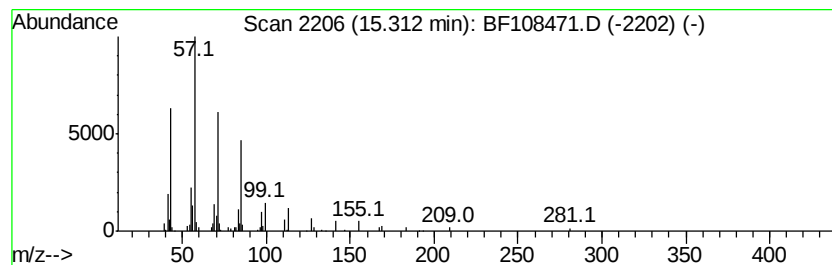
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	2.73 ng	112652	Perylene-d12	15.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Triacontane	422	C30H62	000638-68-6	91
3		Octacosane	394	C28H58	000630-02-4	90
4		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5		Docosane	310	C22H46	000629-97-0	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082418\
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Operator : JU/SJ
Sample : J4581-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q3-B3

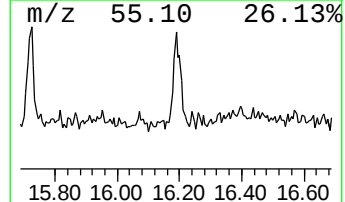
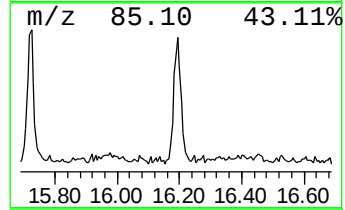
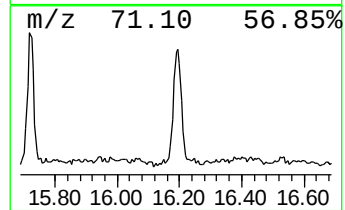
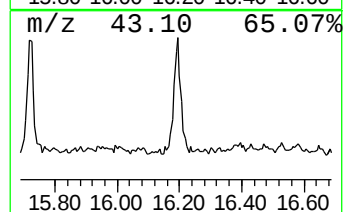
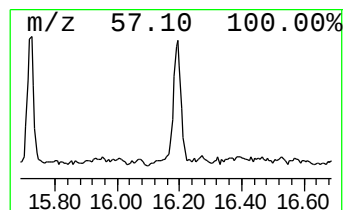
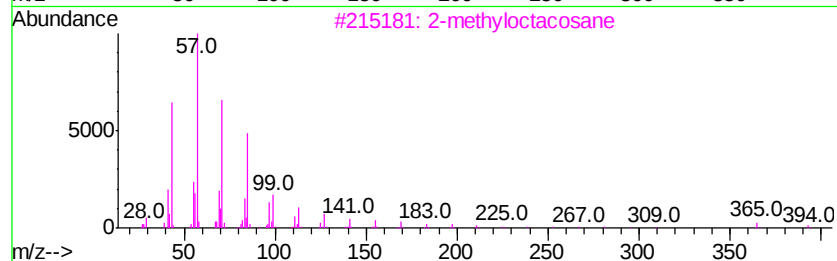
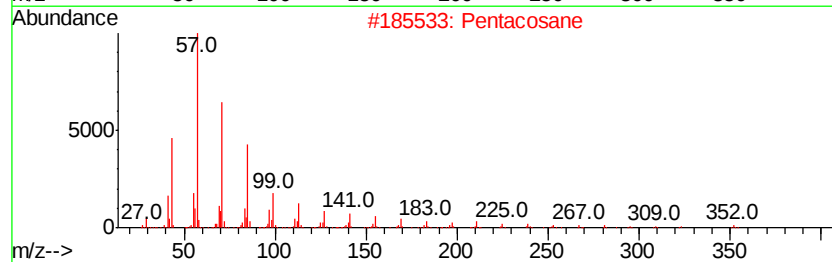
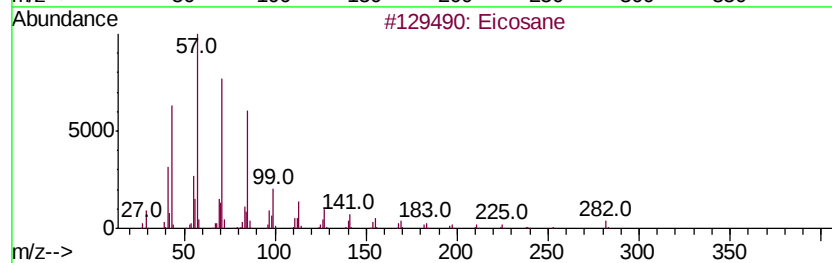
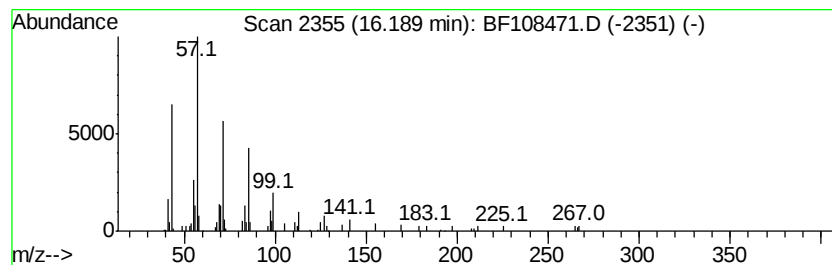
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.90 ng	119855	Perylene-d12	15.74

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	95
2	Pentacosane		352	C25H52	000629-99-2	91
3	2-methyloctacosane		408	C29H60	1000376-72-8	91
4	Heneicosane		296	C21H44	000629-94-7	90
5	Heptacosane		380	C27H56	000593-49-7	90



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Acq On : 24 Aug 2018 18:53
Operator : JU/SJ
Sample : J4581-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q3-B3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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...	2.37	30.5	ng	1179410	1	7.00	772374	20.0
2-Pentanone, 4-hy...	5.25	4.6	ng	178185	1	7.00	772374	20.0
unknown6.77	6.77	78.2	ng	3019020	1	7.00	772374	20.0
Bromoacetic acid,...	14.07	2.1	ng	84776	5	14.19	799386	20.0
Heneicosane	14.32	2.0	ng	81058	5	14.19	799386	20.0
9-Octadecenamide,...	14.94	5.2	ng	208496	5	14.19	799386	20.0
2-methyloctacosane	15.31	2.7	ng	112652	6	15.74	826124	20.0
Eicosane	16.19	2.9	ng	119855	6	15.74	826124	20.0