

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111924\
 Data File : BF140482.D
 Acq On : 19 Nov 2024 19:02
 Operator : RC/JU
 Sample : P4768-03
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-3-3

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-BF111324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140482.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	5	13	26	rVB	1811855	2966575	93.98%	11.293%
2	2.281	26	32	39	rVB	55096	91293	2.89%	0.348%
3	5.099	501	511	525	rBV	100754	169254	5.36%	0.644%
4	5.510	575	581	601	rVB	2090470	2886534	91.44%	10.988%
5	6.510	745	751	769	rBV	2070612	2928359	92.77%	11.148%
6	6.875	807	813	818	rBV	769201	967156	30.64%	3.682%
7	7.434	898	908	917	rBV	1431236	1913236	60.61%	7.283%
8	7.681	946	950	958	rVB	33565	47869	1.52%	0.182%
9	8.151	1011	1030	1036	rBV	915843	1266117	40.11%	4.820%
10	8.563	1097	1100	1107	rVB	27839	36356	1.15%	0.138%
11	8.734	1125	1129	1134	rBV	85354	105103	3.33%	0.400%
12	9.163	1199	1202	1207	rVB	26235	34601	1.10%	0.132%
13	9.228	1207	1213	1221	rBV	2428074	3156669	100.00%	12.017%
14	9.298	1221	1225	1231	rVB	85251	113944	3.61%	0.434%
15	9.563	1266	1270	1273	rVV2	23974	39087	1.24%	0.149%
16	9.622	1276	1280	1287	rVB2	31609	58870	1.86%	0.224%
17	9.833	1311	1316	1320	rVV	69057	87752	2.78%	0.334%
18	9.904	1323	1328	1342	rVB	824614	1116548	35.37%	4.250%
19	10.328	1393	1400	1405	rBV	60870	89583	2.84%	0.341%
20	10.551	1434	1438	1444	rVB	20419	32561	1.03%	0.124%
21	10.622	1444	1450	1456	rVV	413990	540818	17.13%	2.059%
22	10.698	1458	1463	1477	rVV	1101013	1457589	46.17%	5.549%
23	10.804	1477	1481	1490	rVB	63264	112117	3.55%	0.427%
24	10.928	1498	1502	1510	rVB	60568	80104	2.54%	0.305%
25	11.251	1553	1557	1560	rBV	39717	52535	1.66%	0.200%
26	11.398	1576	1582	1590	rBV	744657	1006129	31.87%	3.830%
27	11.680	1626	1630	1634	rVB	32128	38036	1.20%	0.145%
28	11.922	1666	1671	1682	rBV	150236	289367	9.17%	1.102%
29	12.086	1695	1699	1704	rBV2	33986	45951	1.46%	0.175%
30	12.474	1762	1765	1772	rVB2	27642	35404	1.12%	0.135%
31	12.616	1785	1789	1793	rBV	44977	65859	2.09%	0.251%
32	12.710	1801	1805	1810	rBV5	22721	42704	1.35%	0.163%
33	12.845	1824	1828	1835	rVB2	54370	81974	2.60%	0.312%
34	12.980	1846	1851	1861	rBV	1832985	2399810	76.02%	9.136%
35	13.204	1886	1889	1893	rBV	28149	39454	1.25%	0.150%
36	13.463	1927	1933	1942	rBV	348287	506359	16.04%	1.928%

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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-BF111324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.545	1945	1947	1952	rVB	29538	36344	1.15%	0.138%
38	14.045	2027	2032	2042	rBV	531159	757165	23.99%	2.882%
39	15.527	2279	2284	2293	rVB	348710	573575	18.17%	2.183%

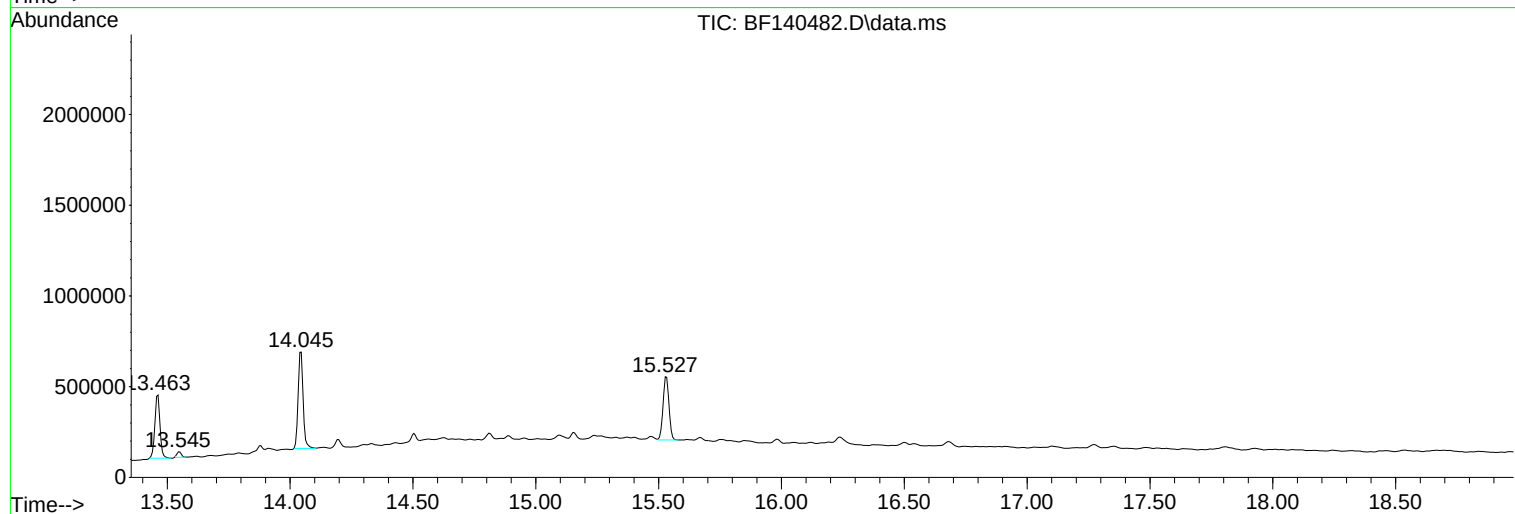
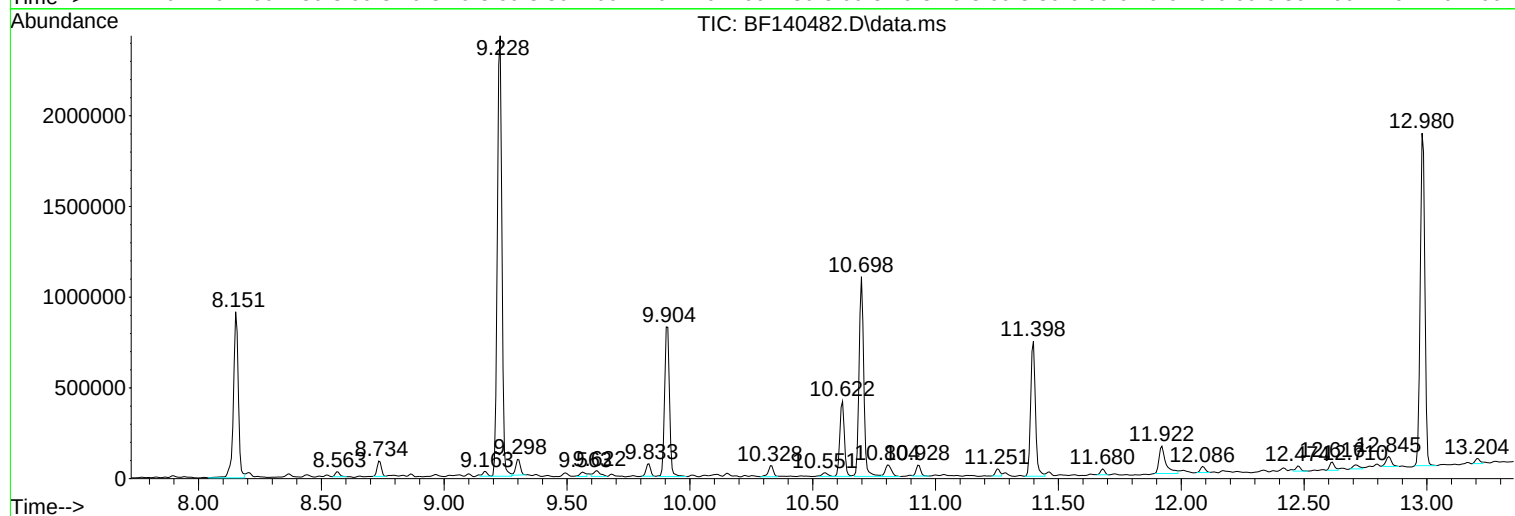
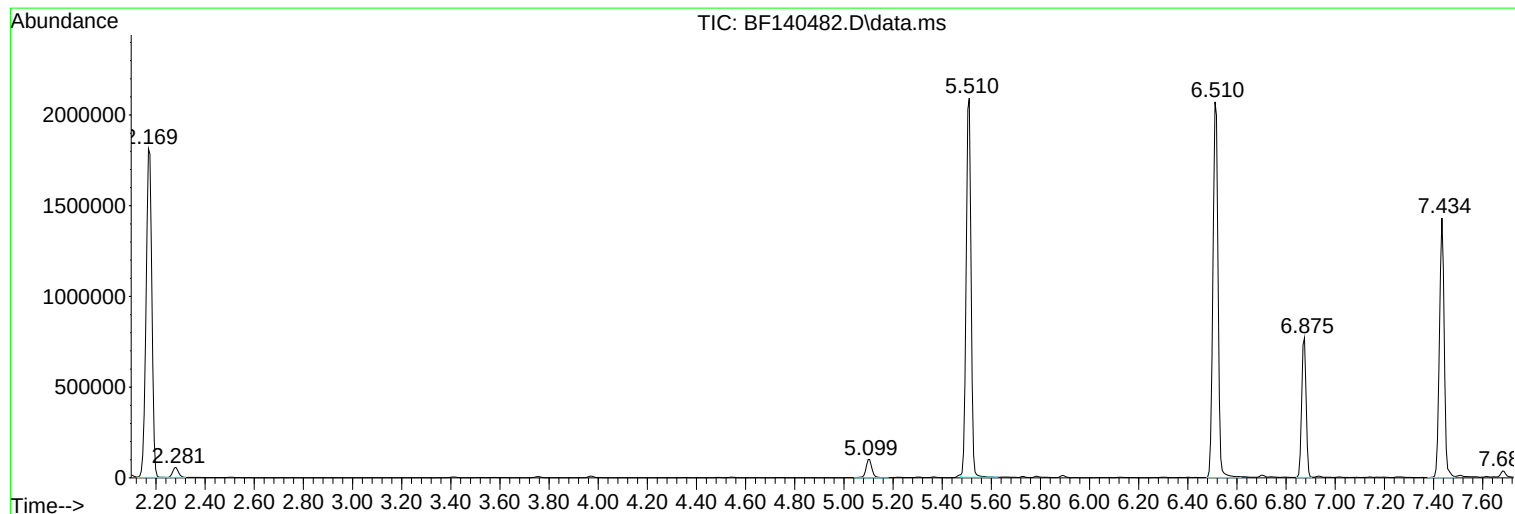
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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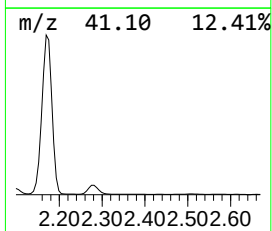
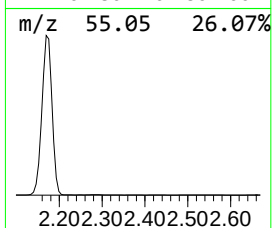
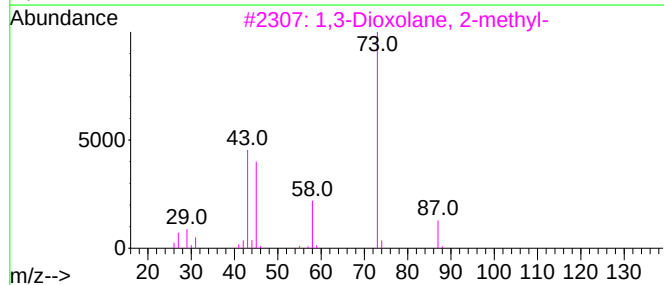
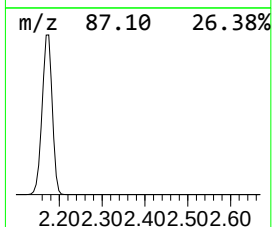
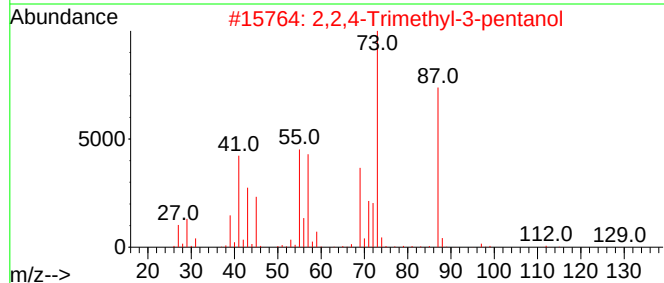
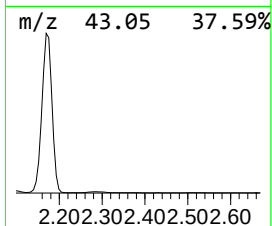
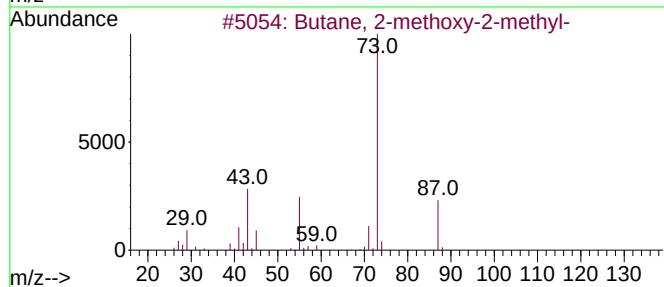
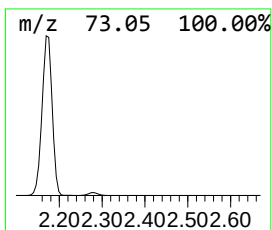
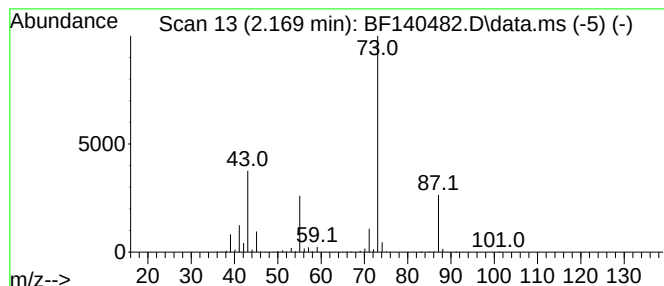
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
2.169	61.35 ng	2966580	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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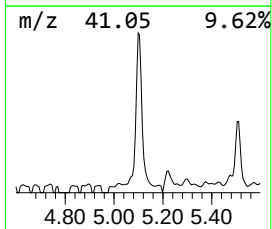
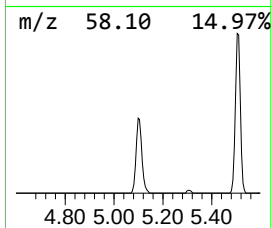
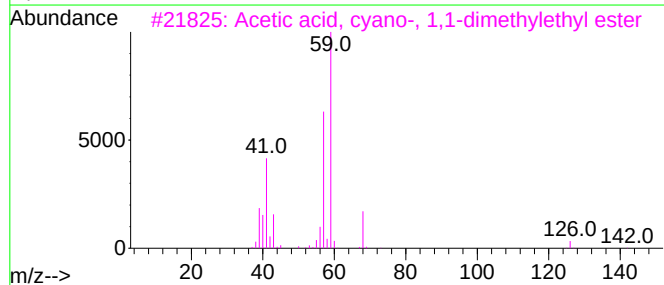
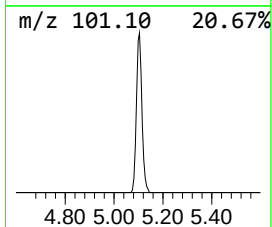
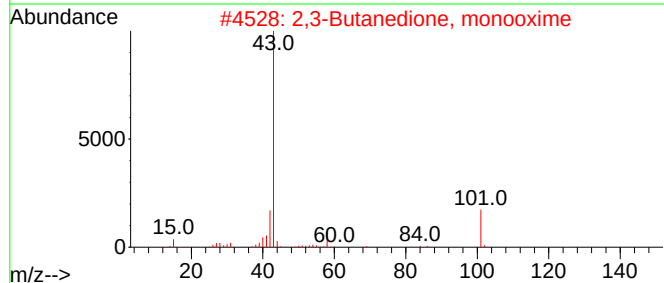
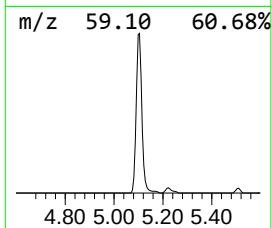
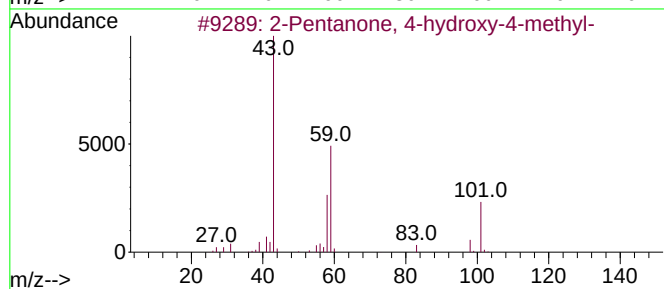
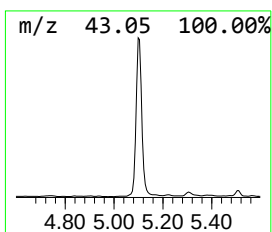
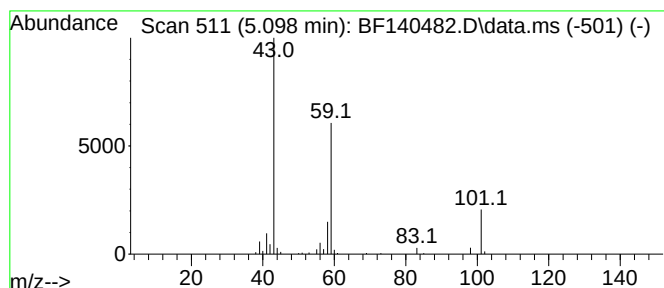
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	3.50 ng	169254	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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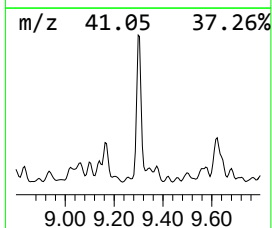
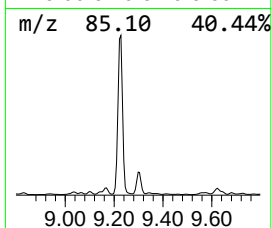
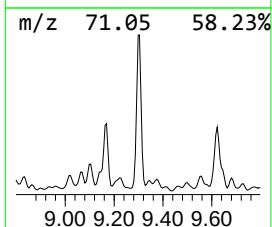
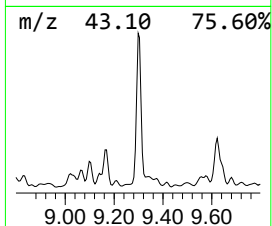
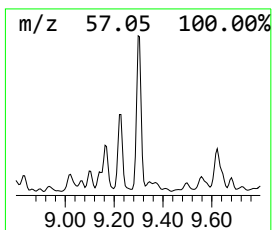
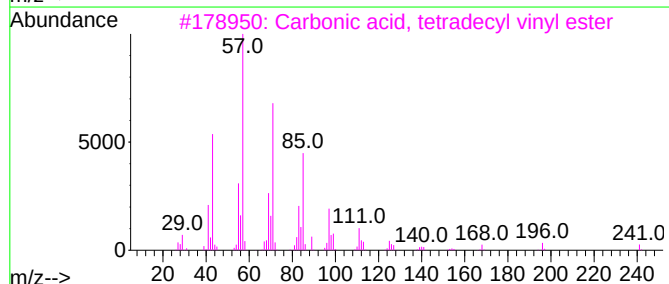
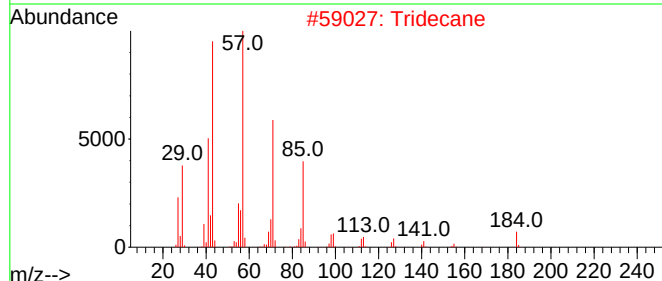
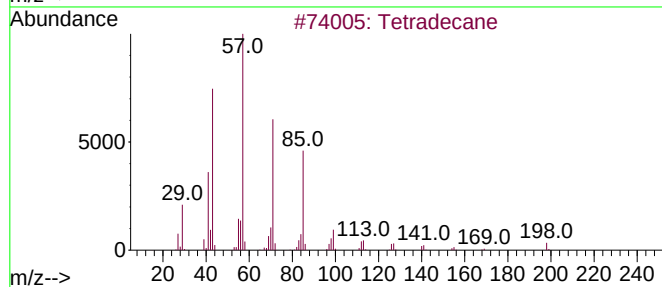
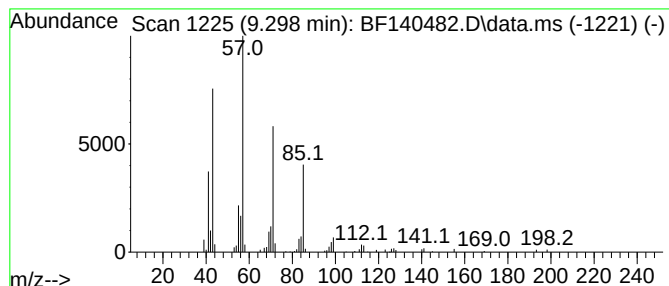
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Tetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.298	2.04 ng	113944	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	97
2			Tridecane	184	C13H28	000629-50-5	90
3			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	83
4			Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	83
5			Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3	78



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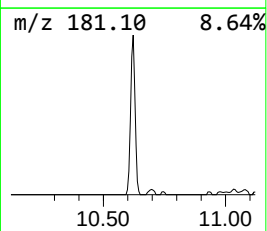
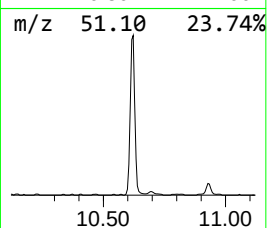
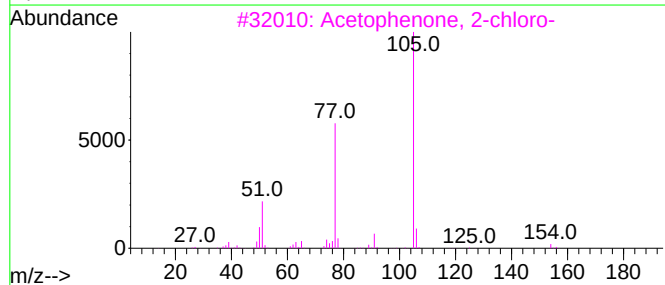
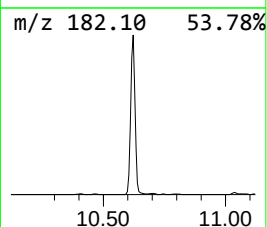
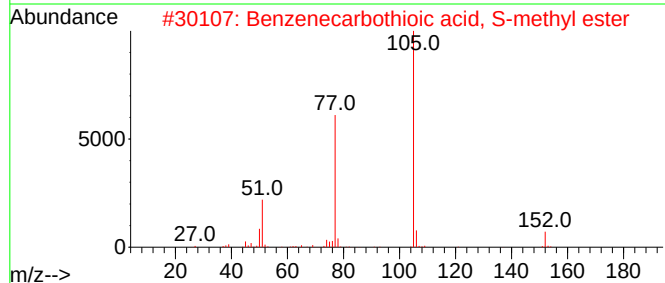
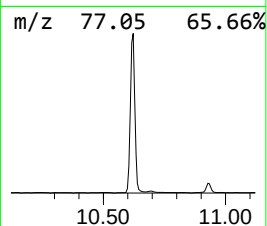
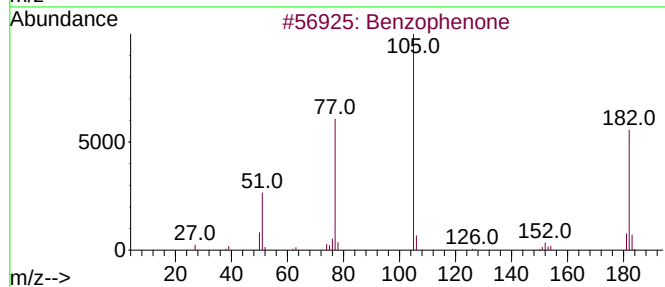
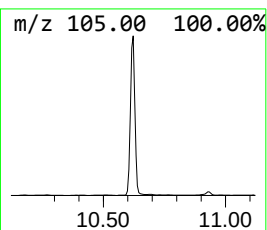
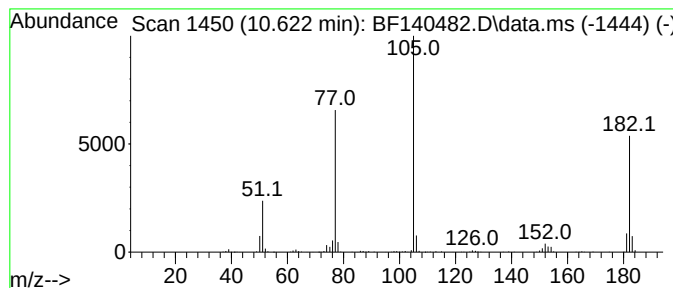
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	9.69 ng	540818	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
5			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47



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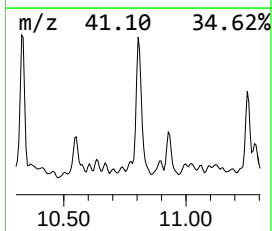
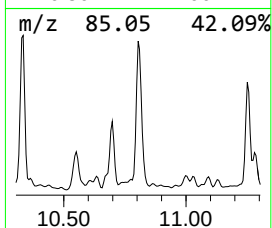
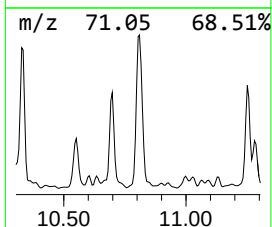
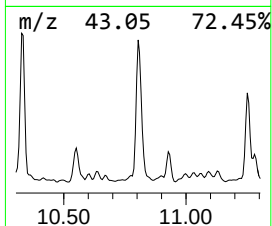
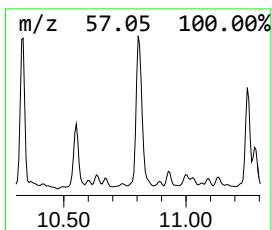
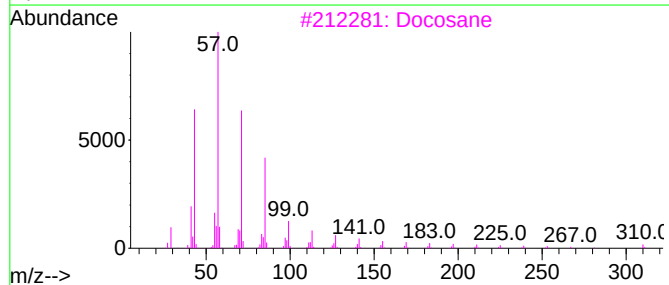
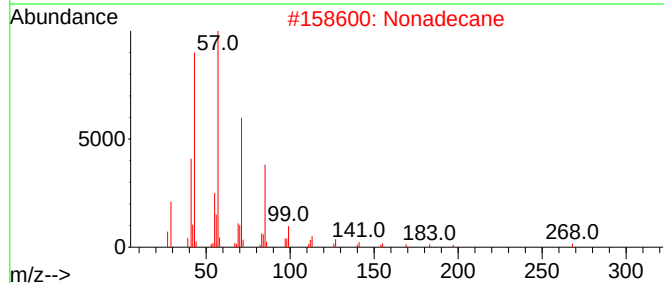
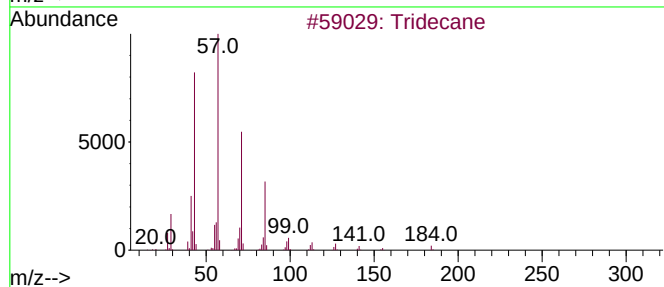
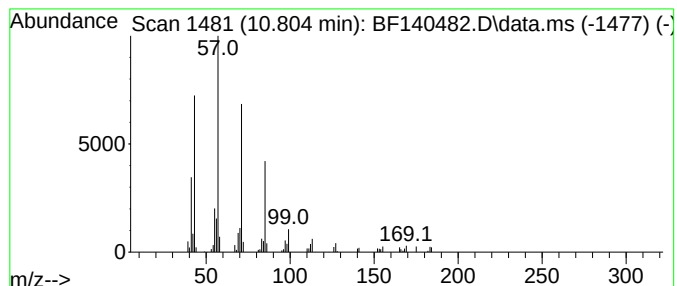
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.804	2.23 ng	112117	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	94
2			Nonadecane	268	C19H40	000629-92-5	91
3			Docosane	310	C22H46	000629-97-0	90
4			Heptacosane	380	C27H56	000593-49-7	90
5			Tetradecane	198	C14H30	000629-59-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111924\
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Acq On : 19 Nov 2024 19:02
Operator : RC/JU
Sample : P4768-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

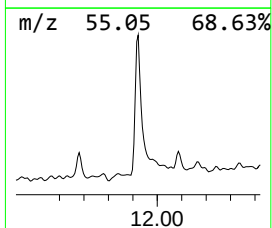
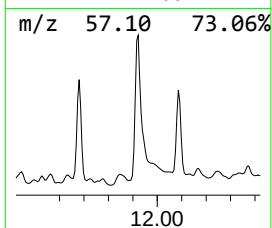
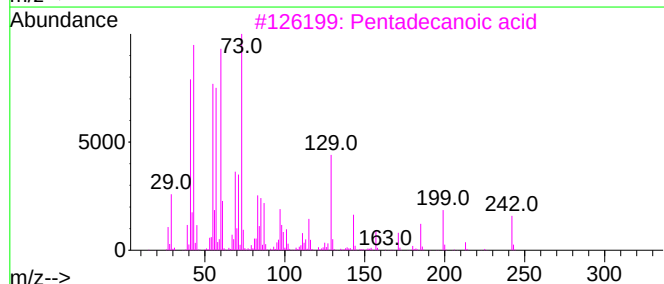
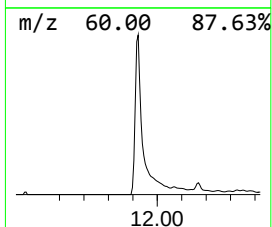
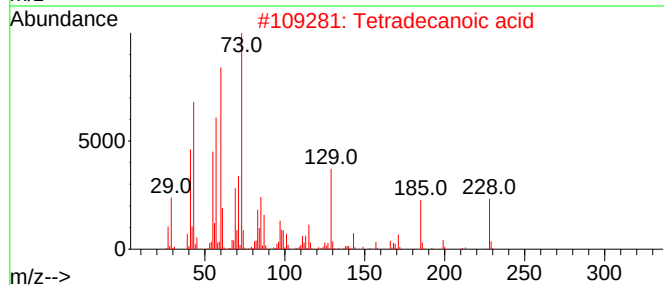
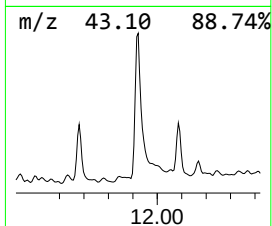
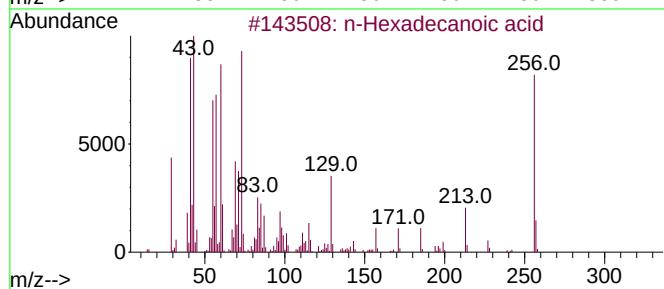
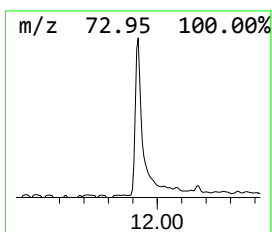
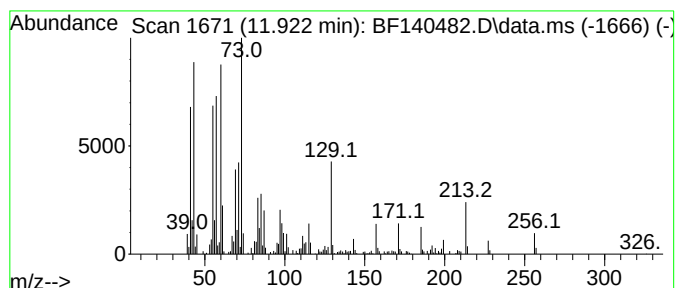
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ClientSampleId :
B-3-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.922	5.75 ng	289367	Phenanthrene-d10		11.398	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid		228	C14H28O2	000544-63-8	94
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	93
4	Undecanoic acid		186	C11H22O2	000112-37-8	83
5	Tridecanoic acid		214	C13H26O2	000638-53-9	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111924\
Data File : BF140482.D
Acq On : 19 Nov 2024 19:02
Operator : RC/JU
Sample : P4768-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-3-3

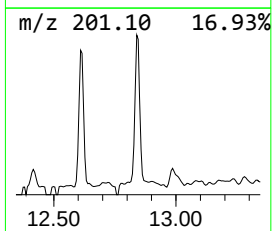
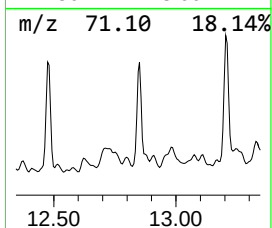
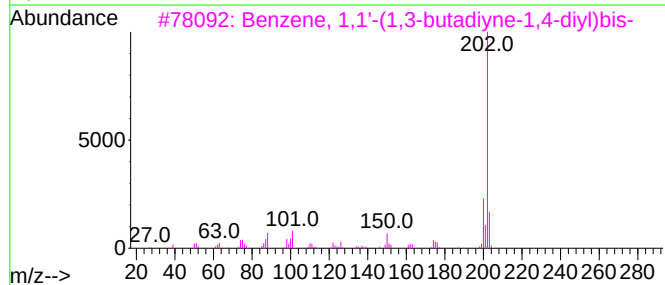
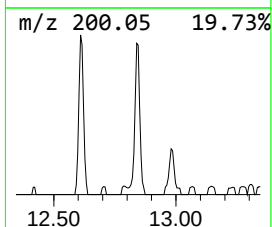
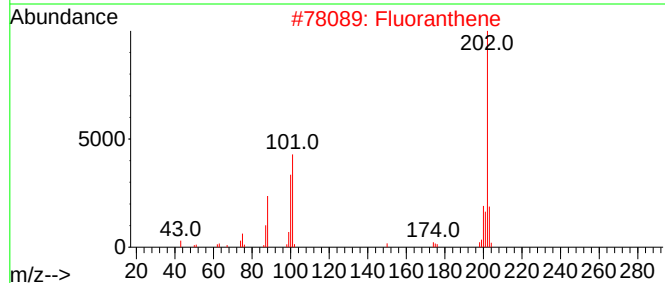
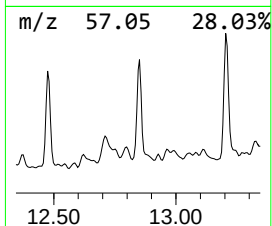
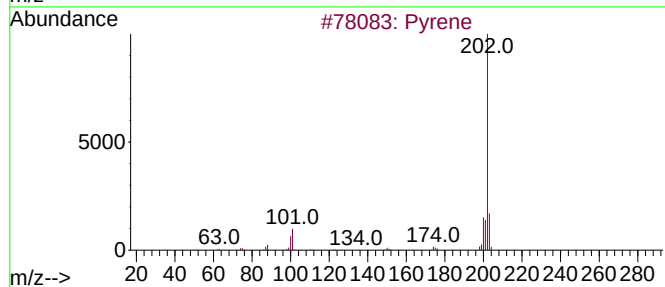
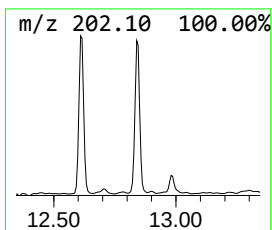
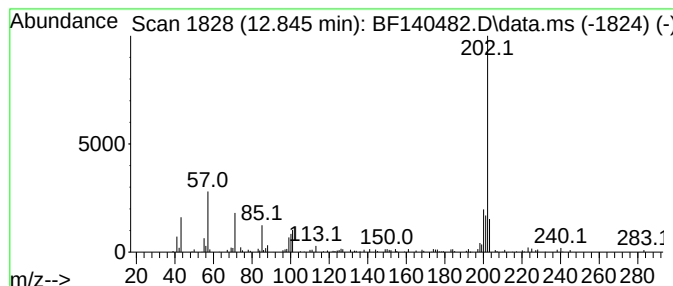
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.845	2.17 ng	81974	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene	202	C16H10	000129-00-0	76
2			Fluoranthene	202	C16H10	000206-44-0	76
3			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	59
4			Acetic acid, 1,2,3-trimethyl-4-p...	261	C16H23NO2	1000271-58-1	40
5			Benzaldehyde, 2,6-difuloro-3,4-d...	202	C9H8F2O3	152434-99-6	36



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111924\
Data File : BF140482.D
Acq On : 19 Nov 2024 19:02
Operator : RC/JU
Sample : P4768-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

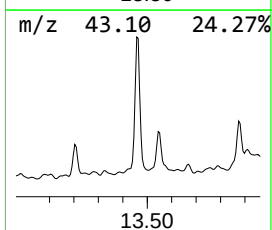
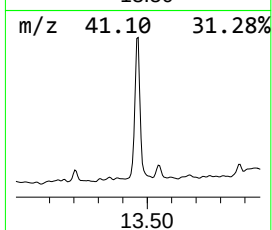
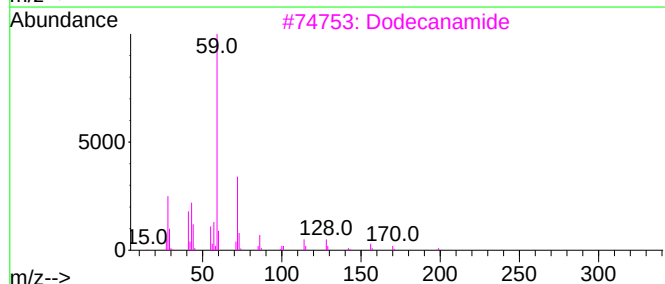
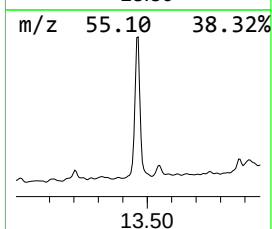
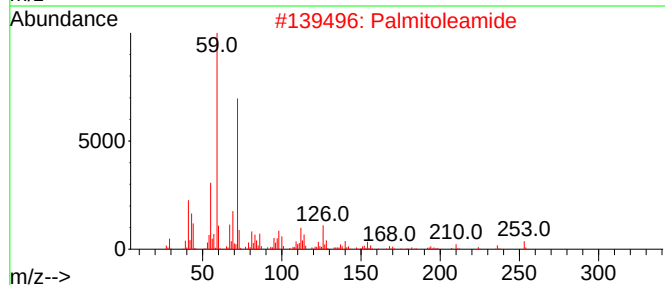
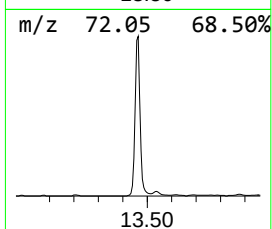
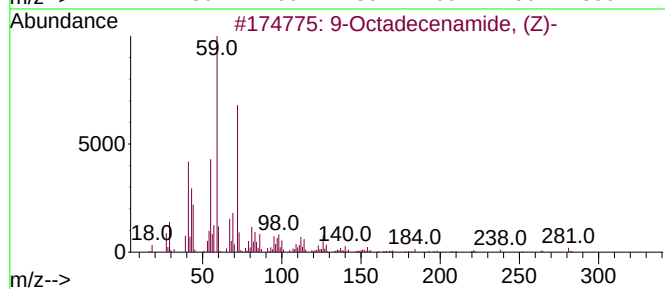
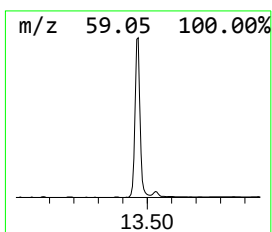
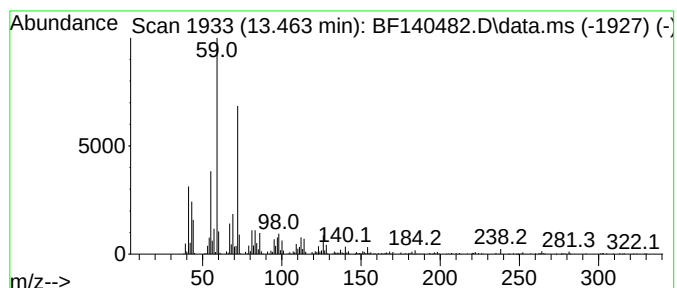
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.463	13.38 ng	506359	Chrysene-d12	14.045	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	Palmitoleamide	253	C16H31NO	106010-22-4	80
3	Dodecanamide	199	C12H25NO	001120-16-7	59
4	Octadecanamide	283	C18H37NO	000124-26-5	59
5	Octanamide	143	C8H17NO	000629-01-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111924\
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Operator : RC/JU
Sample : P4768-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-3-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.169	61.4	ng	2966580	1	6.875	967156	20.0
2-Pentanone, 4-...	5.098	3.5	ng	169254	1	6.875	967156	20.0
Tetradecane	9.298	2.0	ng	113944	3	9.910	1116550	20.0
Benzophenone	10.622	9.7	ng	540818	3	9.910	1116550	20.0
Tridecane	10.804	2.2	ng	112117	4	11.398	1006130	20.0
n-Hexadecanoic ...	11.922	5.8	ng	289367	4	11.398	1006130	20.0
Benzene, 1,1'-(...	12.845	2.2	ng	81974	5	14.045	757165	20.0
9-Octadecenamid...	13.463	13.4	ng	506359	5	14.045	757165	20.0