

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051122\
 Data File : BF128207.D
 Acq On : 11 May 2022 21:14
 Operator : CG\JU
 Sample : N2776-03
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CF-280MER-10-15

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-BF050922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128207.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.504	373	377	385	rBV	172517	192957	8.99%	1.251%
2	5.122	478	482	492	rVB	354398	436064	20.32%	2.827%
3	5.516	545	549	552	rBV	1987933	1887897	87.99%	12.239%
4	6.522	715	720	723	rBV	1919259	1953875	91.07%	12.666%
5	6.892	779	783	786	rBV	602027	497111	23.17%	3.223%
6	7.457	874	879	882	rBV	1413913	1326373	61.82%	8.598%
7	8.175	997	1001	1004	rBV	745672	618604	28.83%	4.010%
8	9.251	1178	1184	1187	rBV	2525298	2145579	100.00%	13.909%
9	9.316	1191	1195	1199	rVB	36372	34370	1.60%	0.223%
10	9.581	1234	1240	1244	rBV3	20708	26184	1.22%	0.170%
11	9.622	1244	1247	1252	rVB3	55956	63002	2.94%	0.408%
12	9.933	1294	1300	1303	rBV	767366	667321	31.10%	4.326%
13	10.722	1430	1434	1445	rBV	1416381	1319516	61.50%	8.554%
14	10.822	1448	1451	1455	rBV3	17043	24684	1.15%	0.160%
15	11.422	1549	1553	1556	rBV	752486	650581	30.32%	4.218%
16	11.445	1556	1557	1562	rVB	110176	65269	3.04%	0.423%
17	11.798	1614	1617	1621	rVB	54773	46143	2.15%	0.299%
18	11.939	1635	1641	1642	rBV2	23923	32280	1.50%	0.209%
19	12.492	1729	1735	1736	rBV3	64904	80702	3.76%	0.523%
20	12.510	1736	1738	1741	rVB	180558	135187	6.30%	0.876%
21	12.592	1750	1752	1756	rBV	28556	25162	1.17%	0.163%
22	12.639	1756	1760	1763	rBV	148337	129419	6.03%	0.839%
23	12.869	1796	1799	1802	rVB	135951	108506	5.06%	0.703%
24	13.010	1818	1823	1826	rBV	1786355	1557522	72.59%	10.097%
25	13.192	1847	1854	1857	rBV	21884	34055	1.59%	0.221%
26	13.557	1913	1916	1920	rBV2	37604	50016	2.33%	0.324%
27	13.780	1951	1954	1956	rBV	35665	32263	1.50%	0.209%
28	14.068	1999	2003	2006	rBV	502835	489741	22.83%	3.175%
29	14.092	2006	2007	2014	rVB	61933	45715	2.13%	0.296%
30	14.163	2016	2019	2023	rVB2	31389	35327	1.65%	0.229%
31	14.515	2077	2079	2083	rVB	31584	26332	1.23%	0.171%
32	15.121	2179	2182	2185	rBV	53772	75543	3.52%	0.490%
33	15.174	2188	2191	2198	rVB2	43926	61699	2.88%	0.400%
34	15.433	2233	2235	2240	rVB	32651	39681	1.85%	0.257%
35	15.498	2243	2246	2252	rVB	52625	66525	3.10%	0.431%
36	15.562	2253	2257	2262	rBV	328936	444543	20.72%	2.882%

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CF-280MER-10-15

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-BF050922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

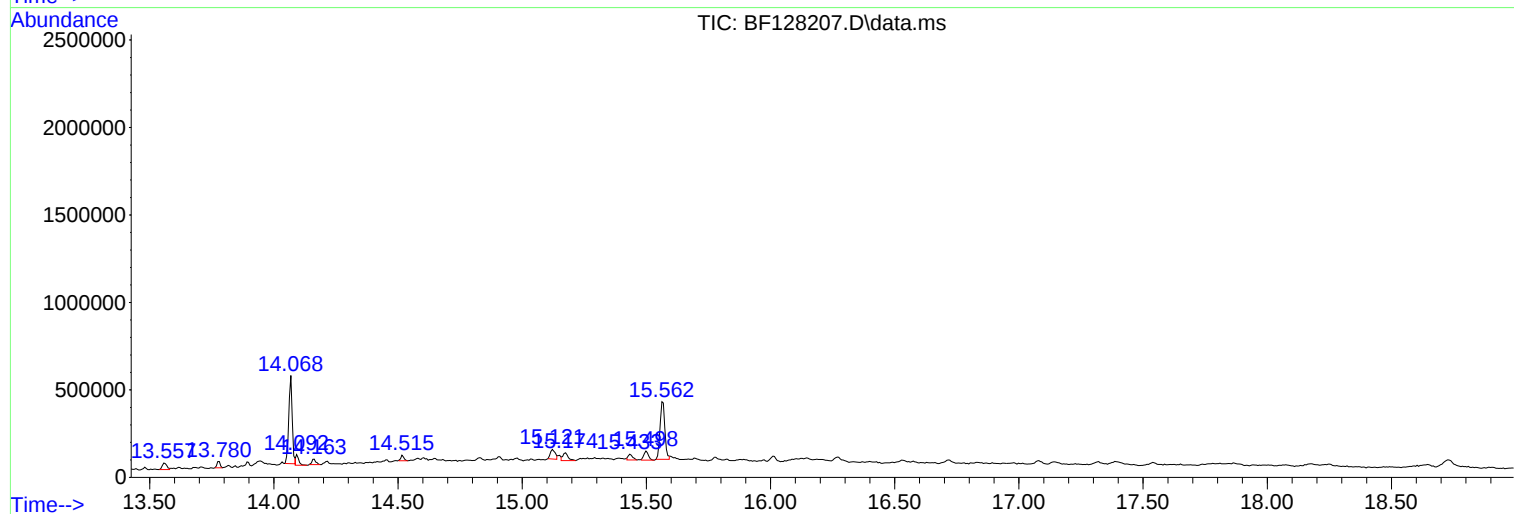
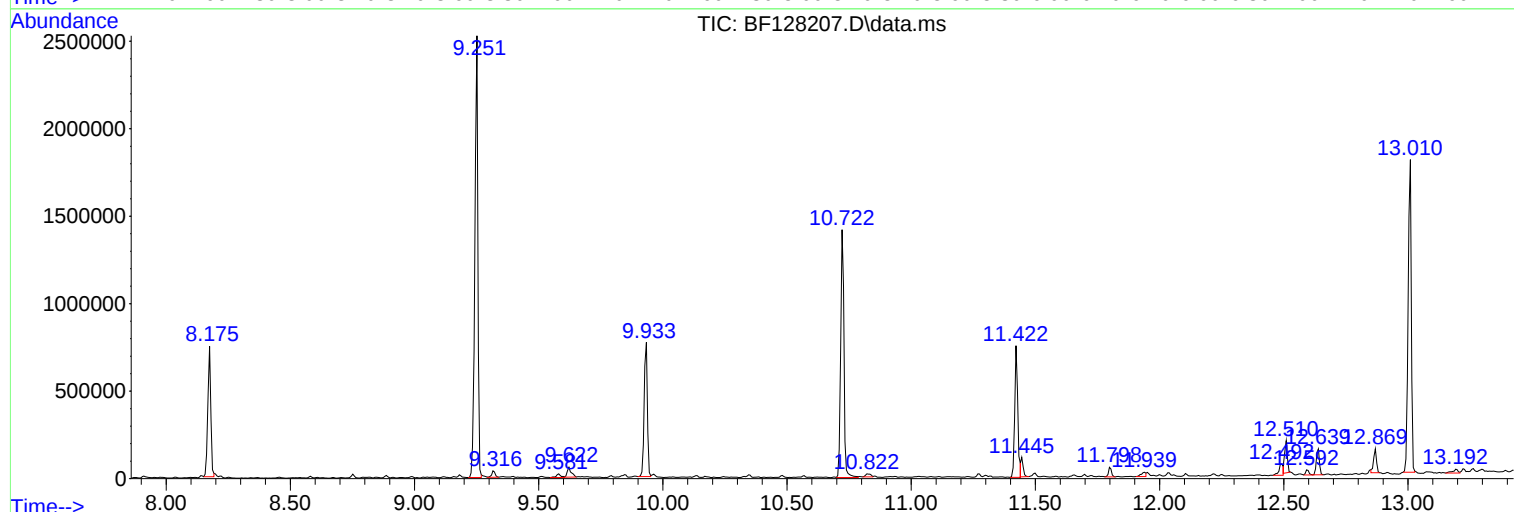
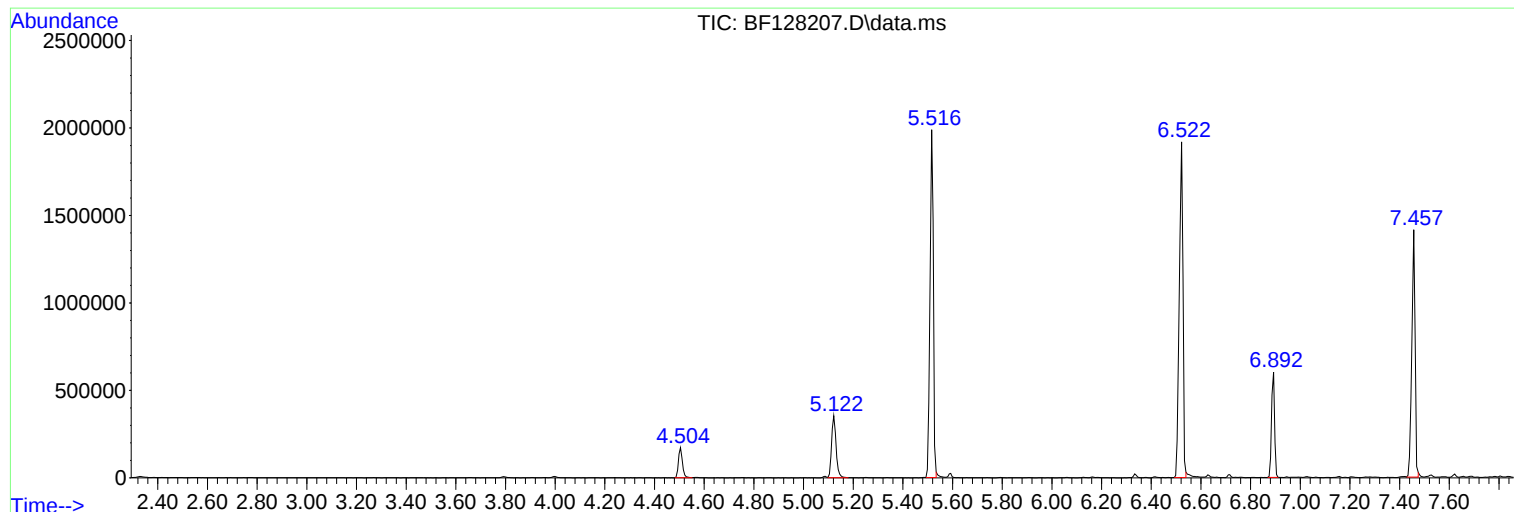
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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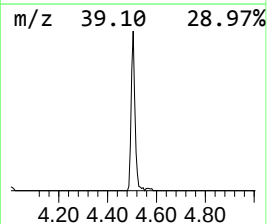
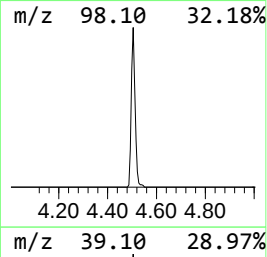
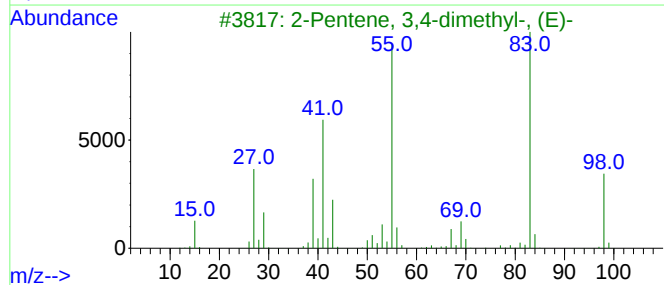
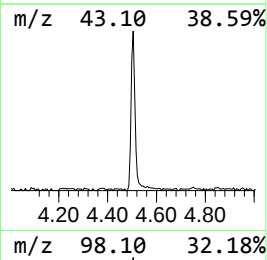
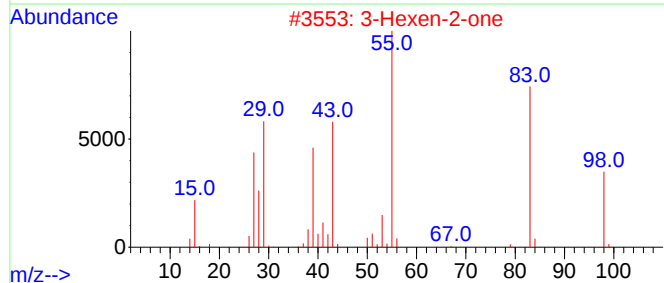
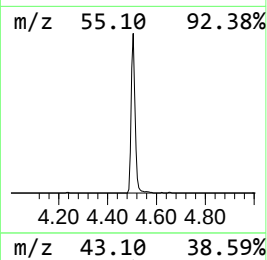
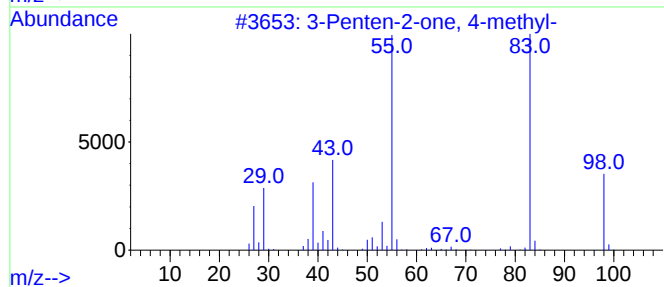
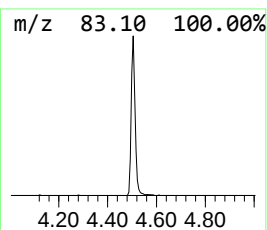
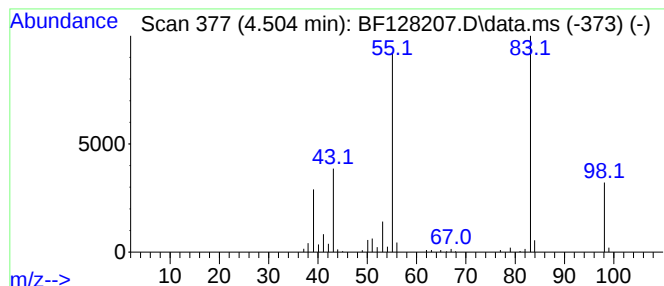
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.504	7.76 ng	192957	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86



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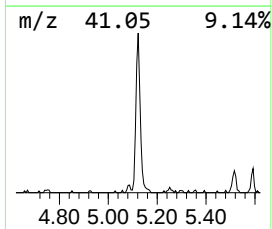
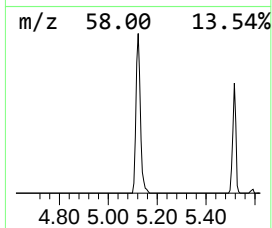
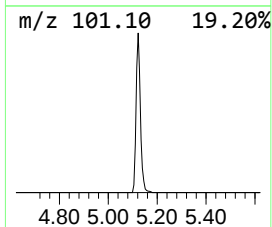
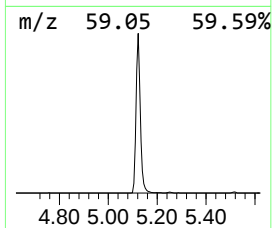
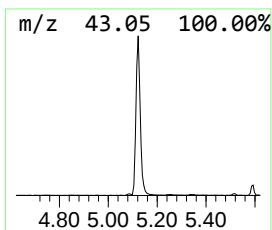
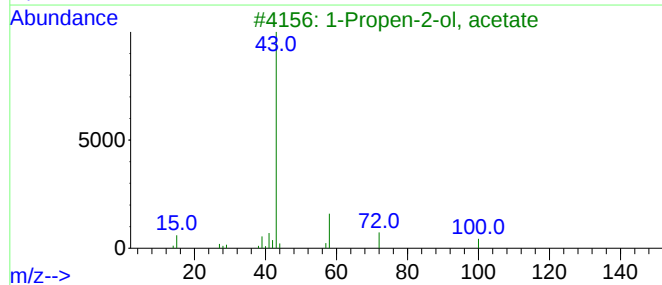
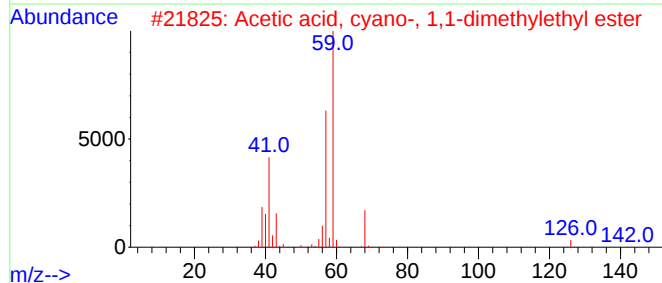
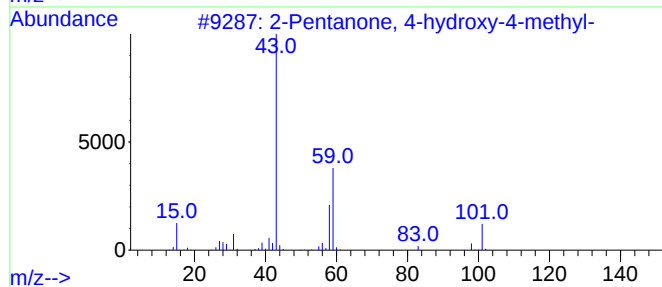
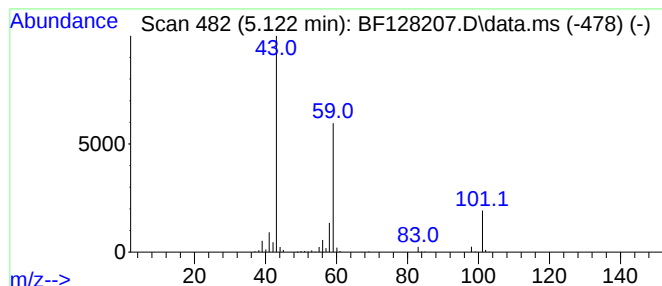
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	17.54 ng	436064	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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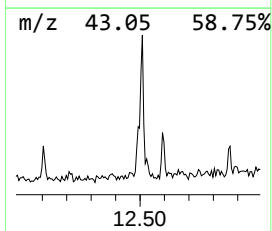
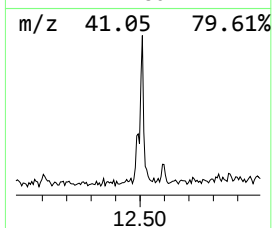
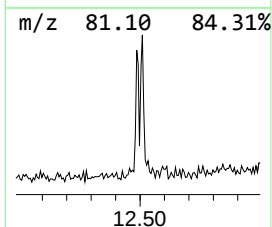
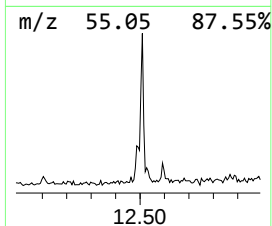
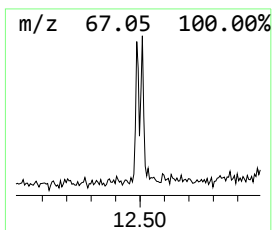
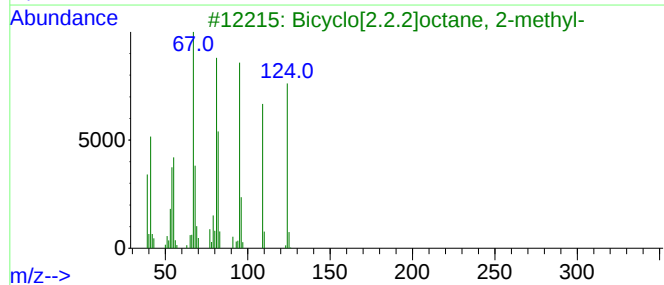
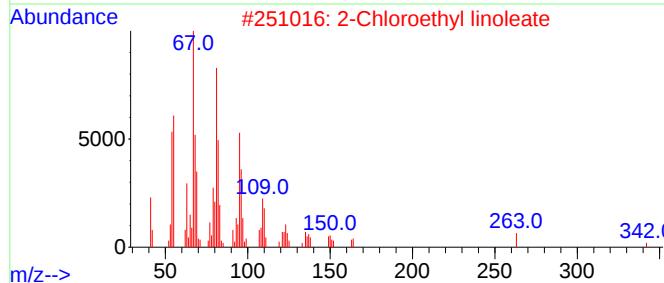
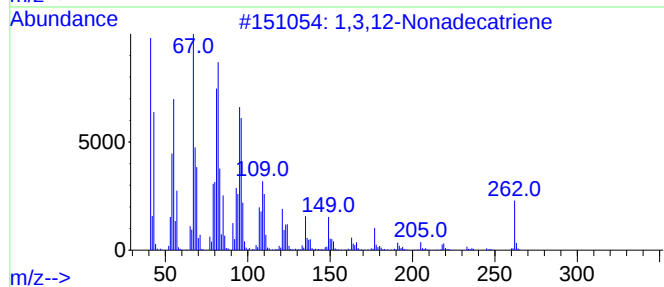
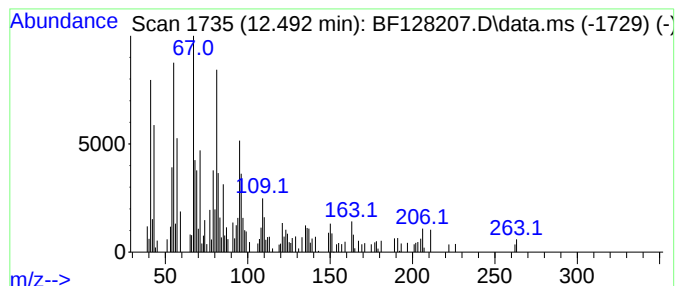
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1,3,12-Nonadecatriene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.492	2.48 ng	80702	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,12-Nonadecatriene		262	C19H34	1000131-11-1	78	
2	2-Chloroethyl linoleate		342	C20H35ClO2	025525-76-2	76	
3	Bicyclo[2.2.2]octane, 2-methyl-		124	C9H16	000766-53-0	68	
4	9,12-Octadecadienoic acid, methyl...		294	C19H34O2	002566-97-4	60	
5	11,14-Eicosadienoic acid, methyl...		322	C21H38O2	002463-02-7	60	



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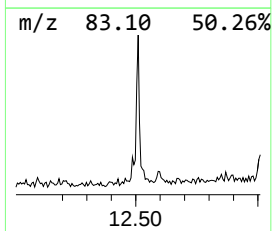
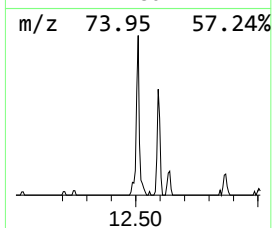
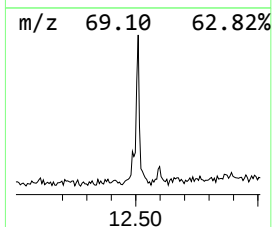
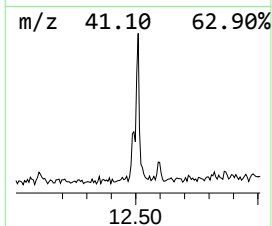
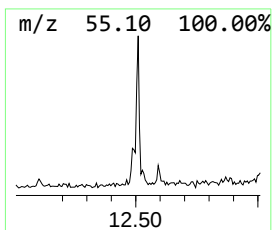
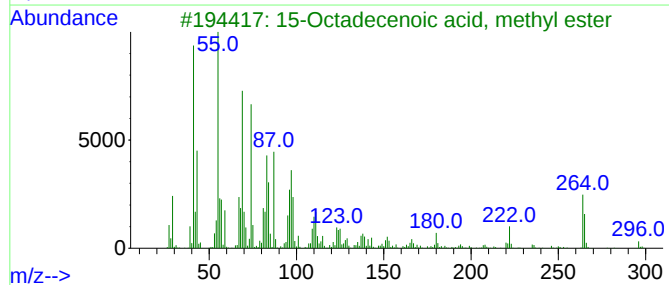
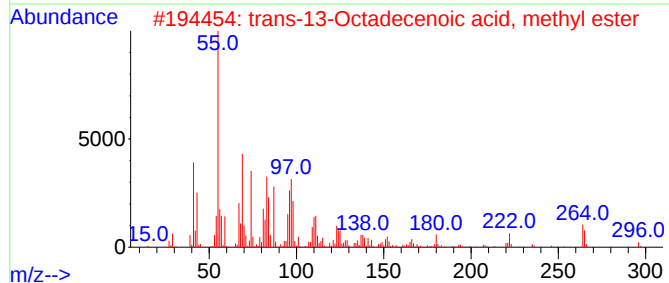
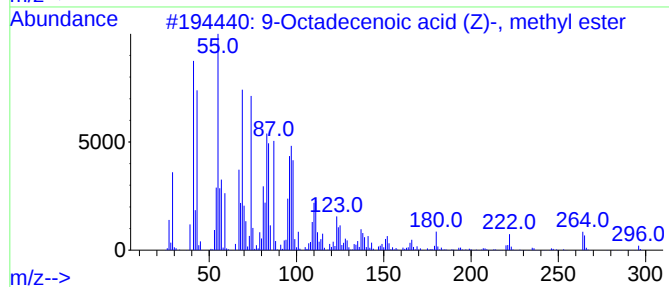
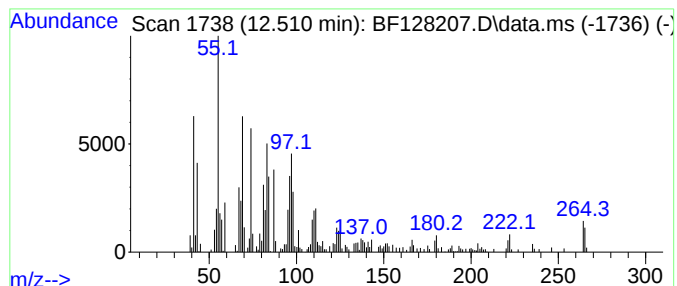
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.510	4.16 ng	135187	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	94
3			15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	91
4			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	87
5			6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	87



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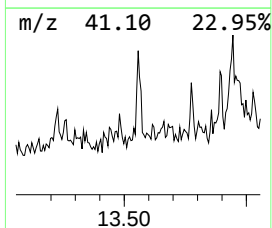
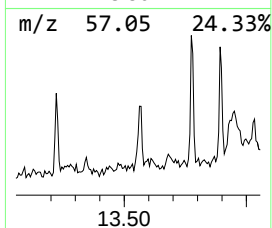
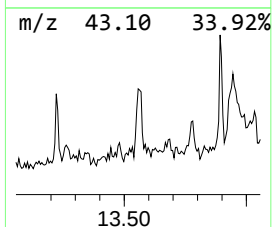
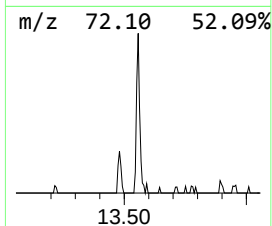
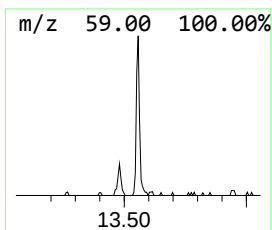
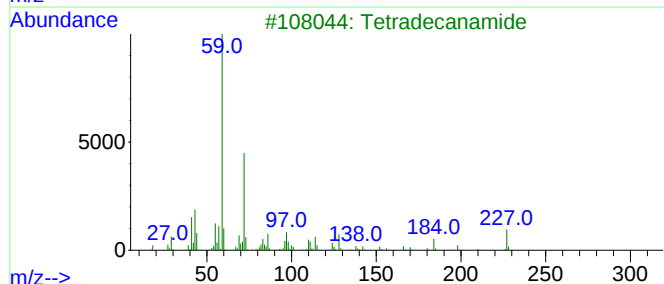
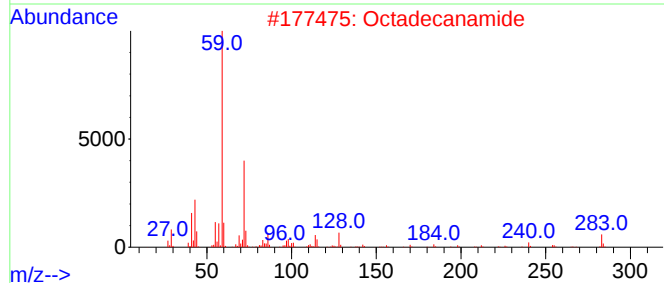
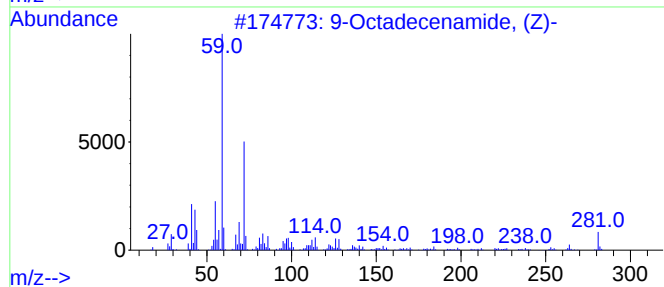
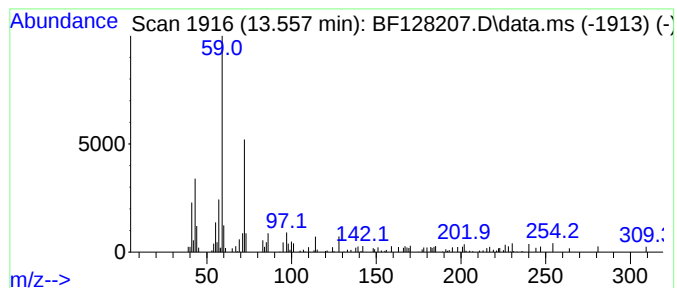
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.557	2.04 ng	50016	Chrysene-d12		14.069	
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-		281	C18H35NO	000301-02-0	93
2	Octadecanamide		283	C18H37NO	000124-26-5	80
3	Tetradecanamide		227	C14H29NO	000638-58-4	72
4	Hexadecanamide		255	C16H33NO	000629-54-9	64
5	Decanamide-		171	C10H21NO	002319-29-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051122\
Data File : BF128207.D
Acq On : 11 May 2022 21:14
Operator : CG\JU
Sample : N2776-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-280MER-10-15

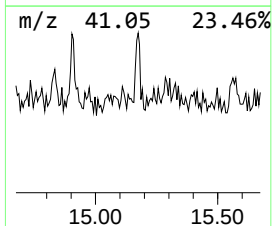
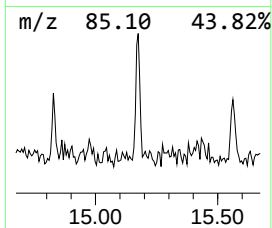
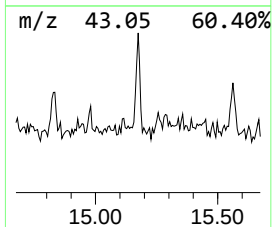
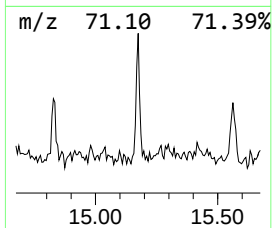
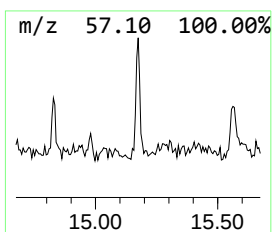
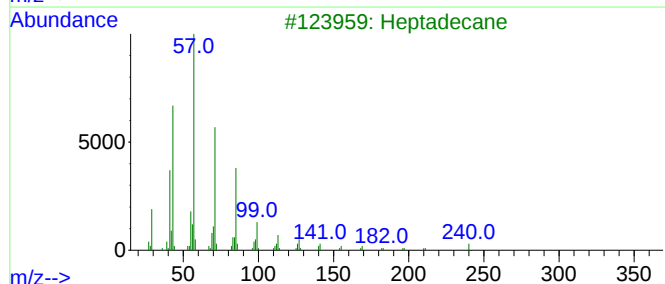
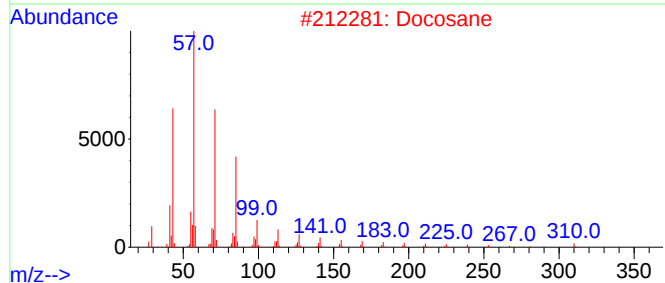
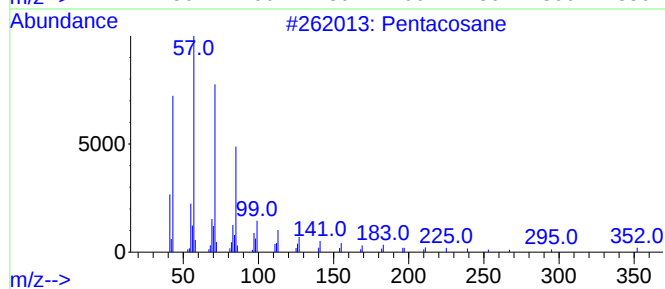
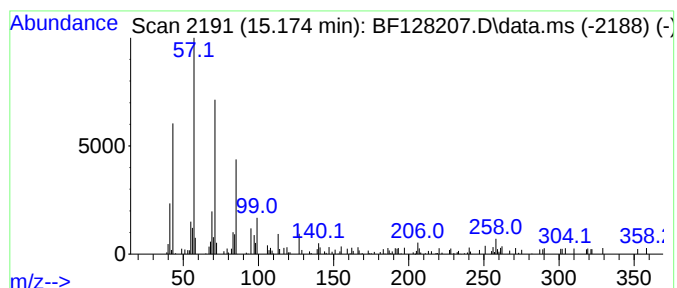
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	2.78 ng	61699	Perylene-d12	15.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	93
2			Docosane	310	C22H46	000629-97-0	93
3			Heptadecane	240	C17H36	000629-78-7	89
4			Octadecane, 5,14-dibutyl-	366	C26H54	055282-13-8	68
5			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051122\
Data File : BF128207.D
Acq On : 11 May 2022 21:14
Operator : CG\JU
Sample : N2776-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-280MER-10-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.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
3-Penten-2-one,...	4.504	7.8	ng	192957	1	6.892	497111	20.0
2-Pentanone, 4-...	5.122	17.5	ng	436064	1	6.892	497111	20.0
1,3,12-Nonadeca...	12.492	2.5	ng	80702	4	11.422	650581	20.0
9-Octadecenoic ...	12.510	4.2	ng	135187	4	11.422	650581	20.0
9-Octadecenamid...	13.557	2.0	ng	50016	5	14.069	489741	20.0
Pentacosane	15.174	2.8	ng	61699	6	15.568	444543	20.0