

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091522\
 Data File : BF130277.D
 Acq On : 15 Sep 2022 18:19
 Operator : CG\JU
 Sample : N4634-04
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-2

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-BF091422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130277.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.869	469	473	486	rVB	327356	452579	12.51%	2.068%
2	5.281	538	543	546	rBV	2580735	2657278	73.43%	12.140%
3	6.310	712	718	721	rBV	2566859	2779914	76.82%	12.700%
4	6.675	776	780	783	rBV	801829	622450	17.20%	2.844%
5	7.240	870	876	879	rBV	1824814	1964705	54.29%	8.976%
6	7.869	980	983	993	rBV	101057	188473	5.21%	0.861%
7	7.957	993	998	1001	rVV	986638	813297	22.47%	3.716%
8	9.034	1176	1181	1184	rBV	3825494	3618950	100.00%	16.533%
9	9.704	1289	1295	1299	rBV	1143503	924444	25.54%	4.223%
10	10.110	1360	1364	1368	rBV3	32818	39770	1.10%	0.182%
11	10.492	1423	1429	1432	rBV	2546126	2124175	58.70%	9.704%
12	10.628	1446	1452	1455	rBV2	47064	65766	1.82%	0.300%
13	11.186	1543	1547	1549	rBV	1074126	870806	24.06%	3.978%
14	11.204	1549	1550	1554	rVB	75519	57055	1.58%	0.261%
15	11.592	1611	1616	1619	rVB	45015	44018	1.22%	0.201%
16	11.716	1633	1637	1641	rVB2	53264	60961	1.68%	0.279%
17	12.392	1748	1752	1756	rBV	90022	87712	2.42%	0.401%
18	12.616	1785	1790	1793	rBV	66979	63402	1.75%	0.290%
19	12.774	1812	1817	1820	rBV	3395392	2907339	80.34%	13.282%
20	13.351	1909	1915	1918	rBV2	38643	41878	1.16%	0.191%
21	13.680	1964	1971	1977	rVB2	37586	45186	1.25%	0.206%
22	13.810	1989	1993	1996	rBV	559233	526454	14.55%	2.405%
23	14.574	2119	2123	2131	rBV2	107599	148527	4.10%	0.679%
24	14.904	2175	2179	2185	rVB2	41653	47527	1.31%	0.217%
25	15.204	2225	2230	2236	rBV	398614	455310	12.58%	2.080%
26	15.645	2301	2305	2310	rBV2	36061	52519	1.45%	0.240%
27	16.698	2478	2484	2492	rVB2	128229	228256	6.31%	1.043%

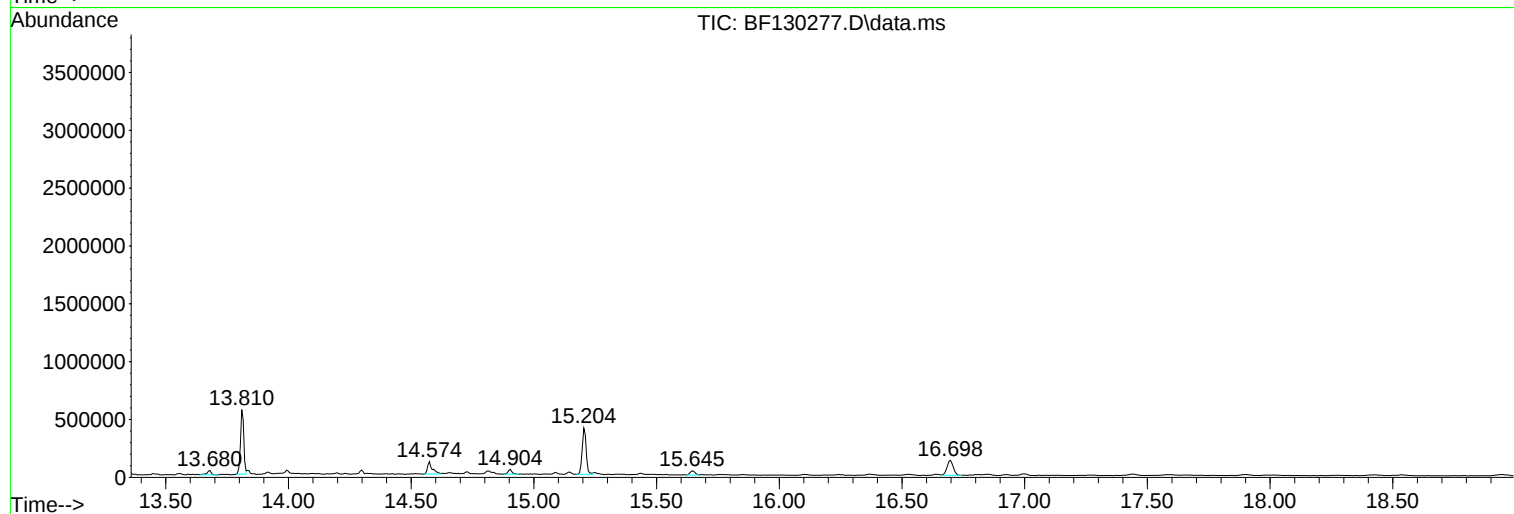
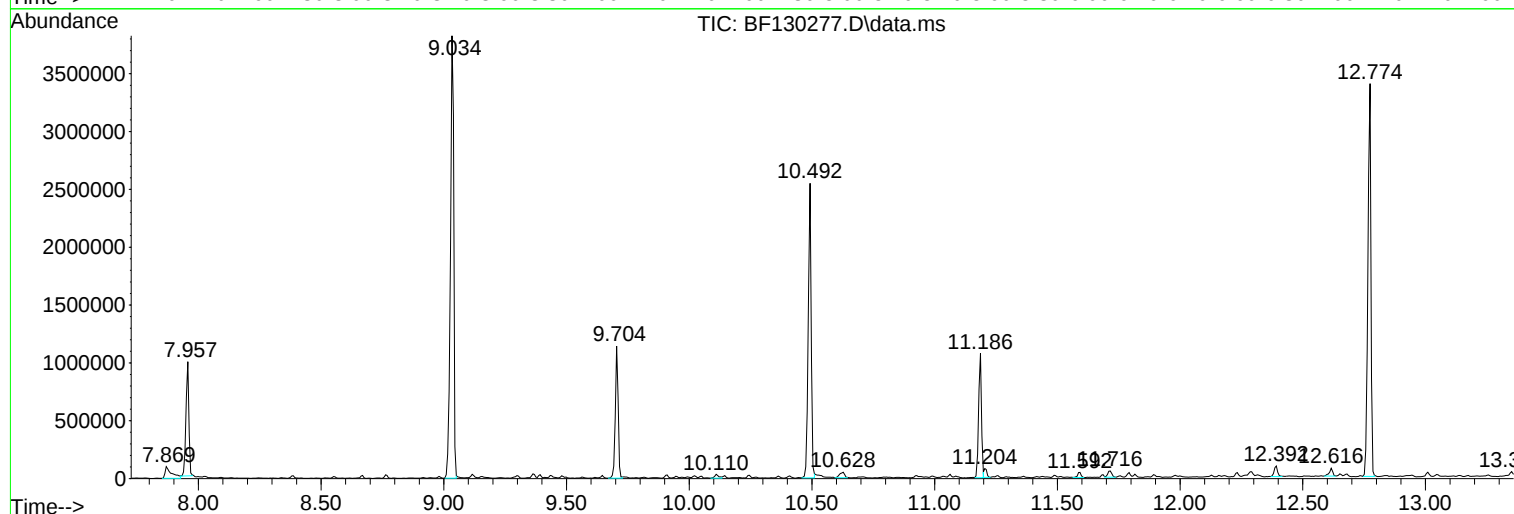
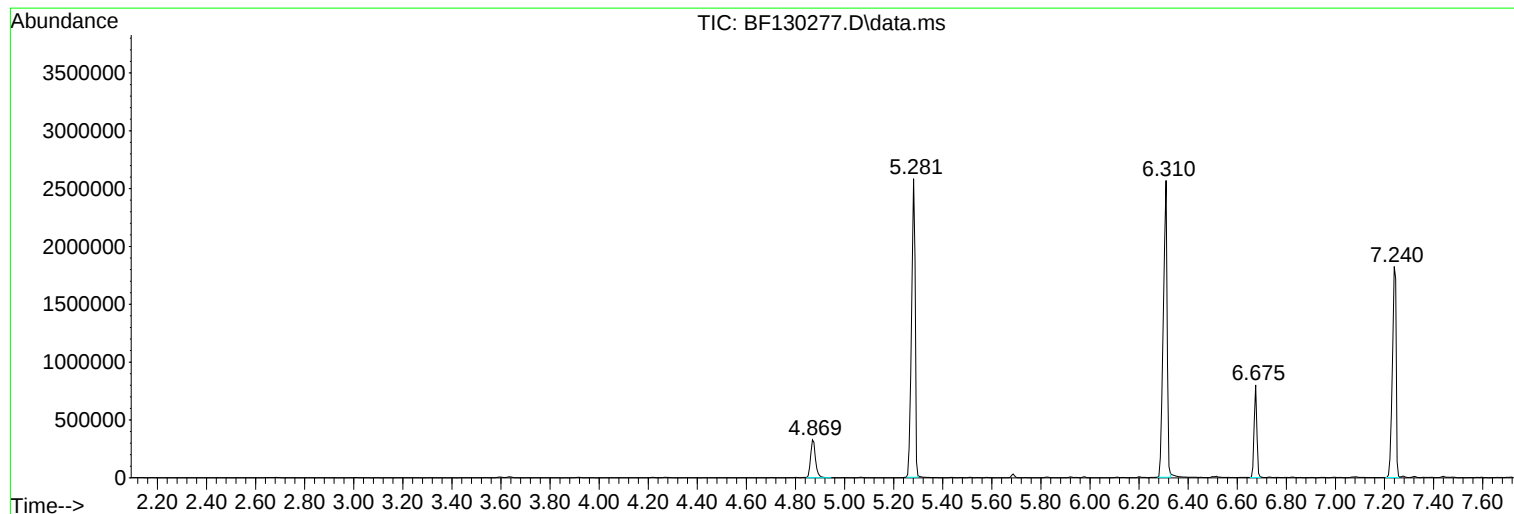
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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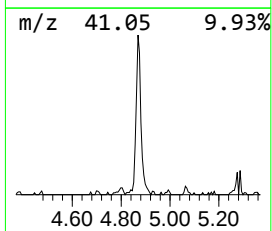
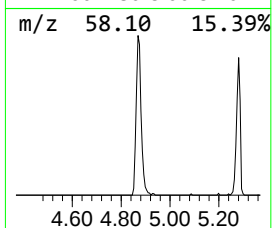
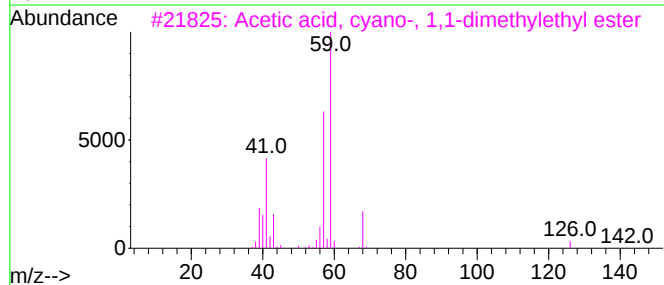
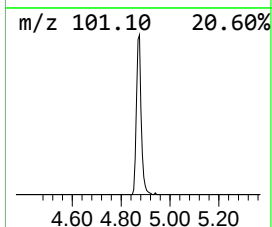
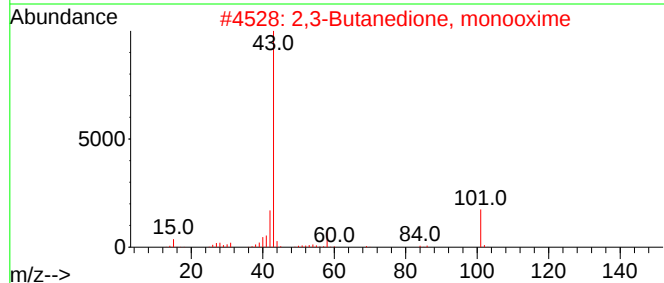
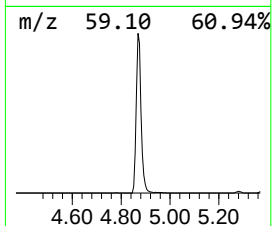
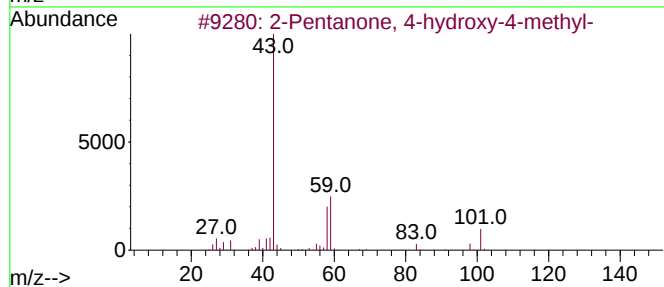
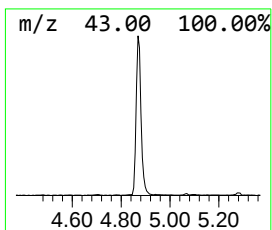
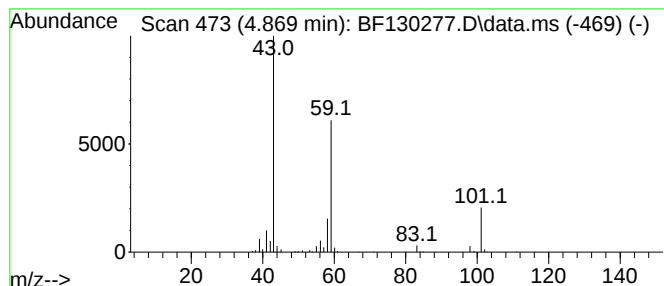
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.869	14.54 ng	452579	1,4-Dichlorobenzene-d4	6.675

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	23		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



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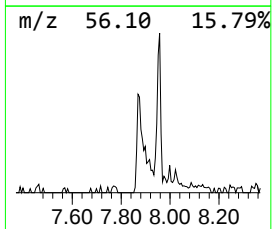
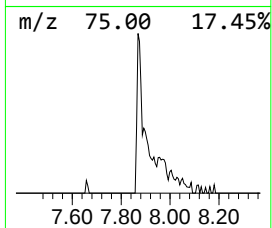
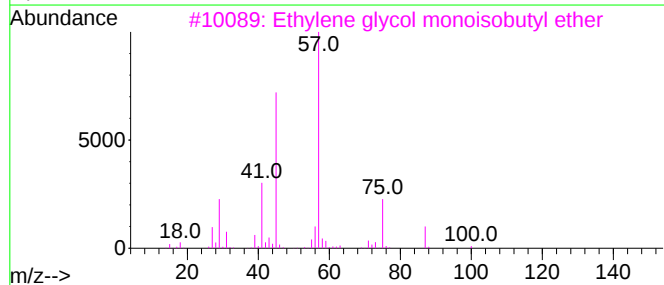
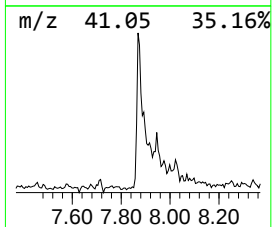
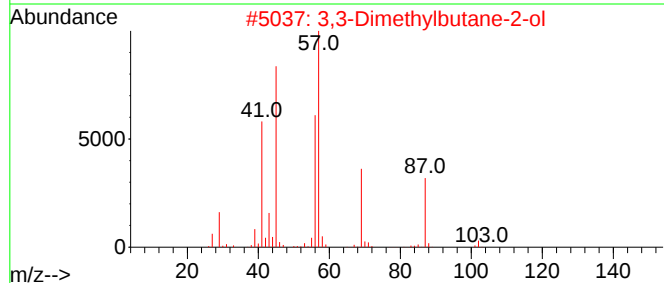
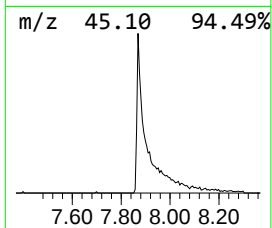
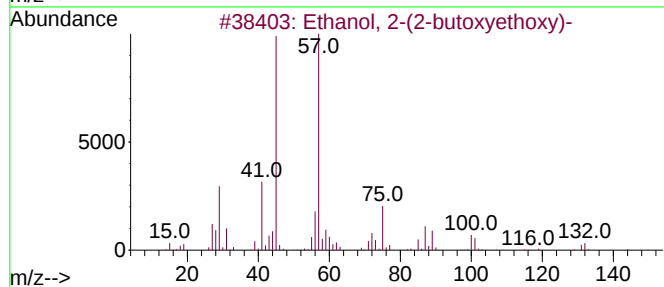
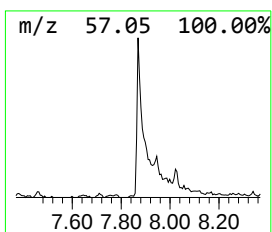
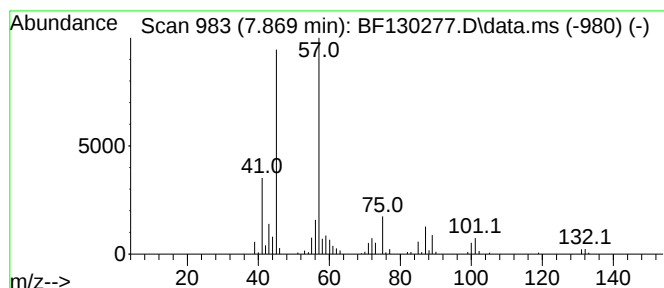
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.869	4.63 ng	188473	Naphthalene-d8	7.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
4			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



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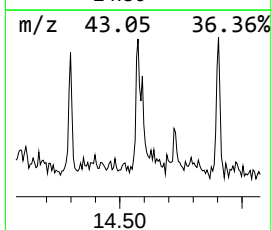
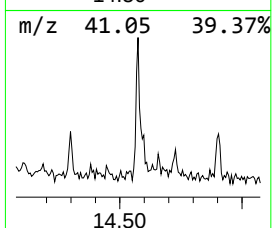
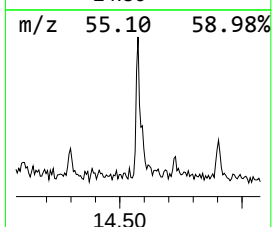
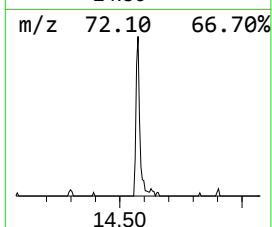
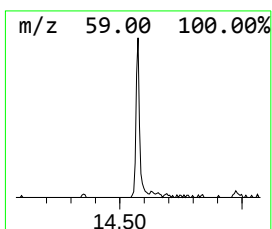
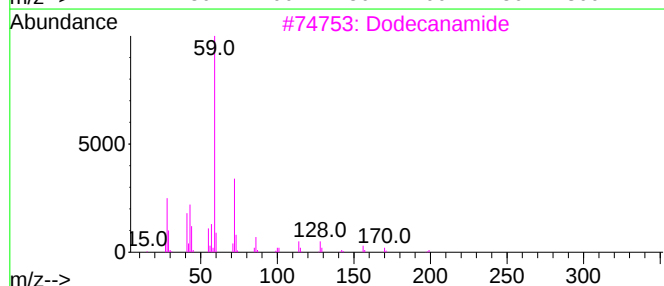
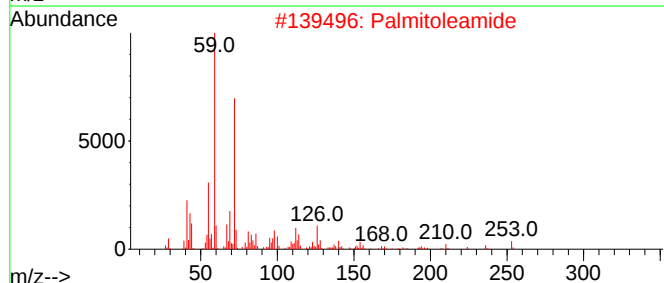
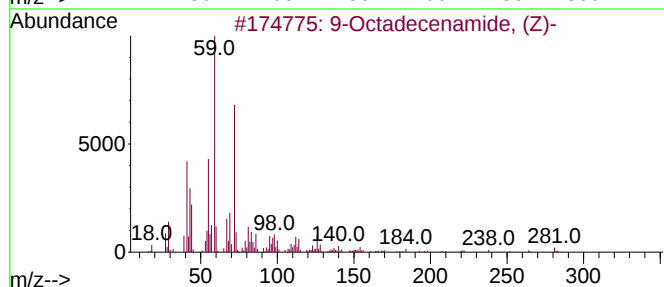
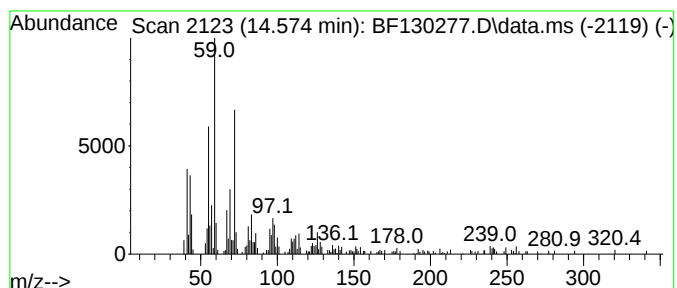
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.574	6.52 ng	148527	Perylene-d12	15.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
2			Palmitoleamide	253	C16H31NO	106010-22-4	86
3			Dodecanamide	199	C12H25NO	001120-16-7	60
4			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	58
5			7-Nonenamide	155	C9H17NO	090949-53-4	53



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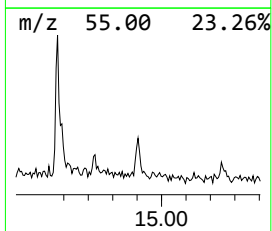
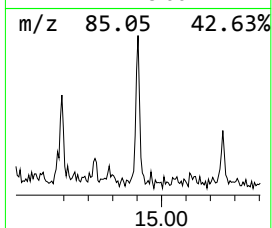
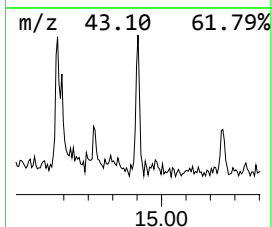
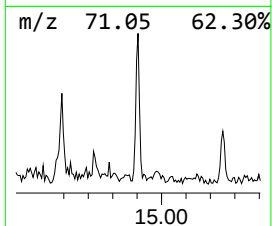
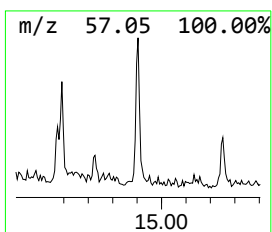
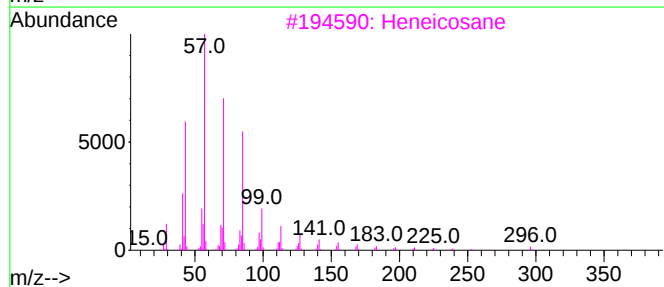
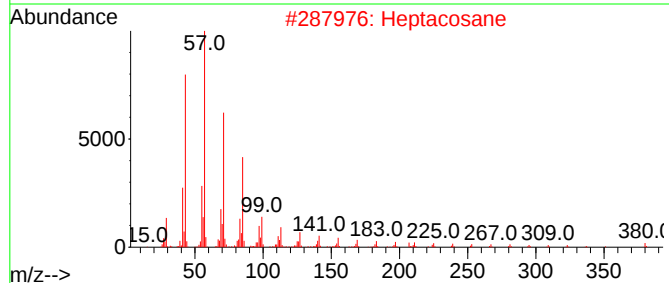
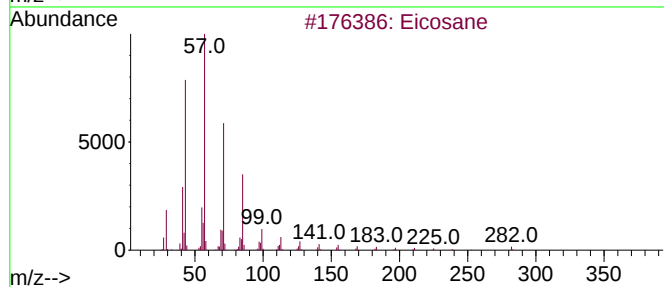
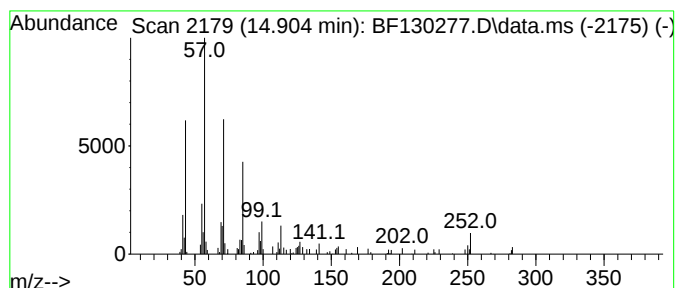
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Peak Number 6 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.904	2.09 ng	47527	Perylene-d12	15.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Heptacosane	380	C27H56	000593-49-7	87
3			Heneicosane	296	C21H44	000629-94-7	87
4			Pentacosane	352	C25H52	000629-99-2	83
5			Tetracosane	338	C24H50	000646-31-1	83



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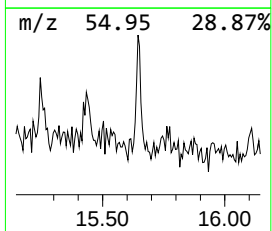
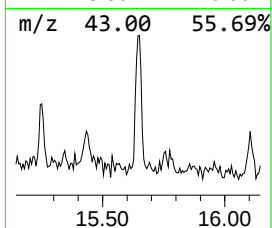
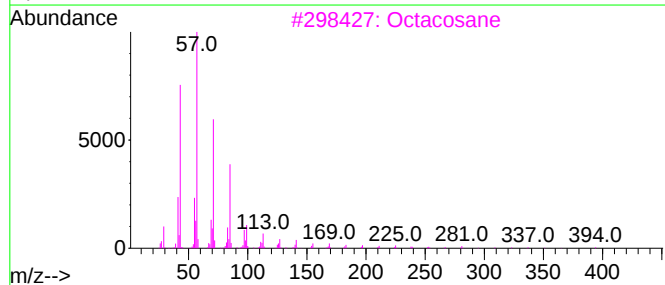
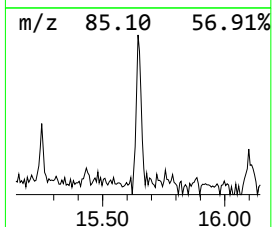
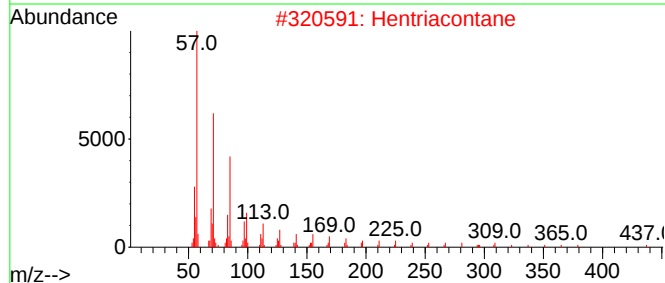
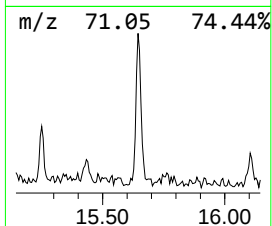
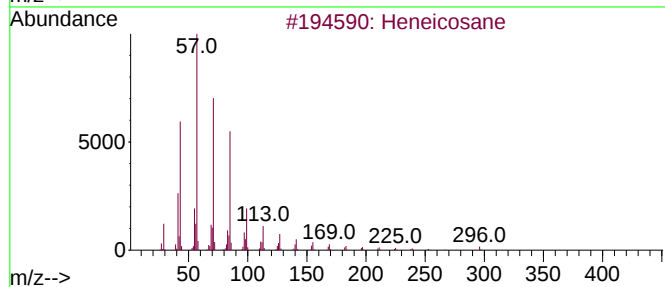
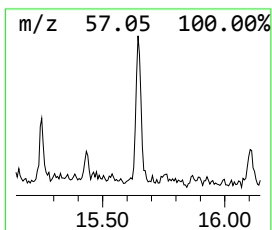
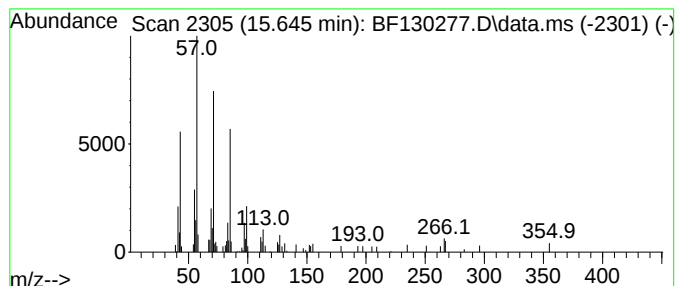
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TIC Library : C:\Database\NIST20.L
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Peak Number 7 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.645	2.31 ng	52519	Perylene-d12	15.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	94
2			Hentriacontane	437	C31H64	000630-04-6	90
3			Octacosane	394	C28H58	000630-02-4	87
4			Hexacosane	366	C26H54	000630-01-3	87
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	86



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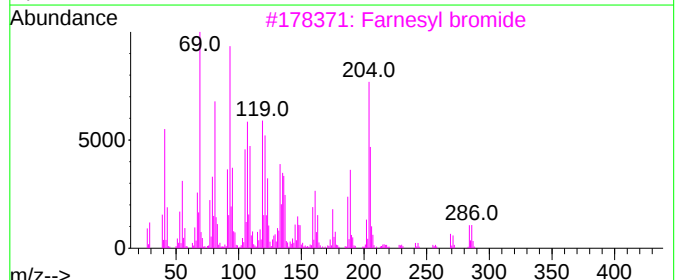
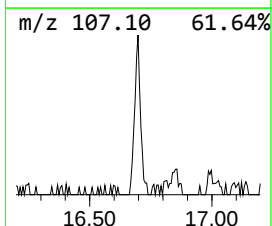
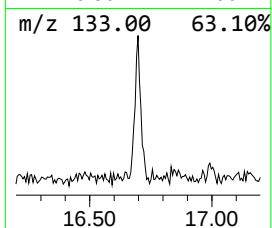
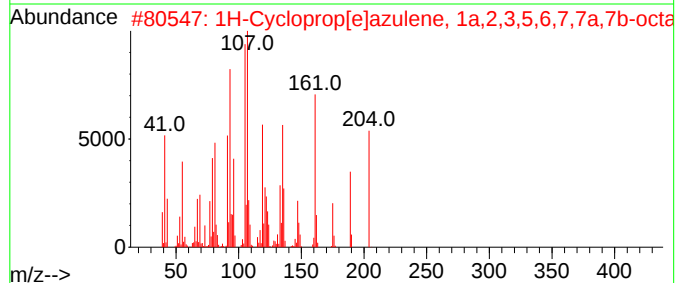
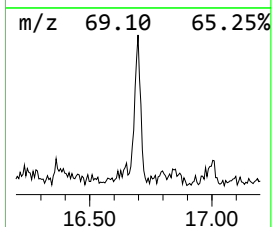
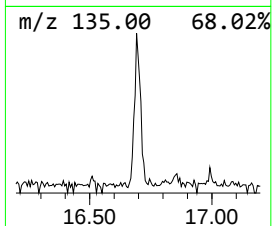
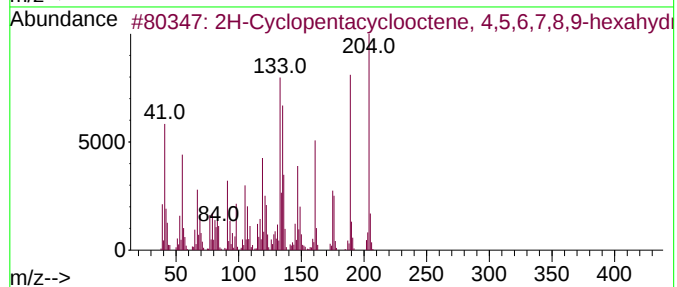
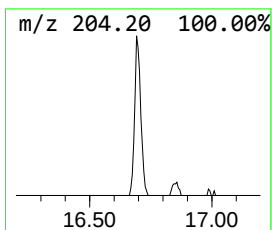
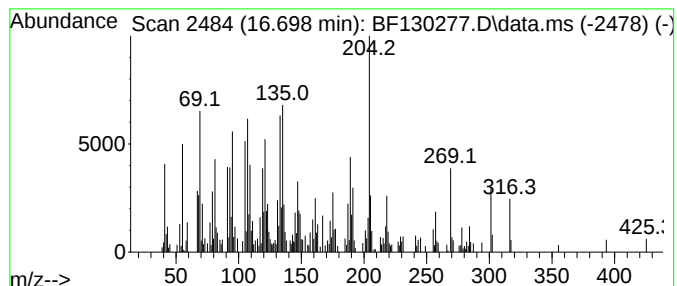
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2H-Cyclopentacyclooctene, 4... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.698	10.03 ng	228256	Perylene-d12	15.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-Cyclopentacyclooctene, 4,5,6,...	204	C15H24	1000221-85-8	64
2			1H-Cycloprop[e]azulene, 1a,2,3,5...	204	C15H24	021747-46-6	52
3			Farnesyl bromide	284	C15H25Br	006874-67-5	49
4			2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	46
5			Alloaromadendrene	204	C15H24	025246-27-9	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091522\
Data File : BF130277.D
Acq On : 15 Sep 2022 18:19
Operator : CG\JU
Sample : N4634-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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
2-Pentanone, 4-...	4.869	14.5	ng	452579	1	6.675	622450	20.0
Ethanol, 2-(2-b...	7.869	4.6	ng	188473	2	7.957	813297	20.0
9-Octadecenamid...	14.574	6.5	ng	148527	6	15.204	455310	20.0
Eicosane	14.904	2.1	ng	47527	6	15.204	455310	20.0
Heneicosane	15.645	2.3	ng	52519	6	15.204	455310	20.0
2H-Cyclopentacy...	16.698	10.0	ng	228256	6	15.204	455310	20.0