

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
 Data File : BF125633.D
 Acq On : 24 Sep 2021 21:52
 Operator : JU/CG
 Sample : M3911-16
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P287-DITCH

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-BF092421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125633.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	13	21	26	rVB	3390878	4583689	69.39%	11.921%
2	5.504	576	581	584	rBV	2551435	2531005	38.32%	6.582%
3	6.498	745	750	753	rBV	1914049	1608827	24.36%	4.184%
4	6.886	812	816	819	rBV	1365639	1131874	17.14%	2.944%
5	7.445	905	911	914	rBV	3345292	3378030	51.14%	8.785%
6	8.063	1012	1016	1023	rBV	193771	169714	2.57%	0.441%
7	8.163	1029	1033	1037	rBV	1641580	1594141	24.13%	4.146%
8	9.245	1211	1217	1220	rBV	6679739	6605260	100.00%	17.178%
9	9.921	1327	1332	1335	rBV	2203411	1843672	27.91%	4.795%
10	10.010	1344	1347	1350	rVB	129878	92268	1.40%	0.240%
11	10.710	1459	1466	1469	rBV	4087934	3848568	58.27%	10.009%
12	11.404	1580	1584	1588	rBV	2116982	1781662	26.97%	4.634%
13	11.927	1670	1673	1677	rBV2	183096	159472	2.41%	0.415%
14	12.710	1803	1806	1811	rBV	72296	75588	1.14%	0.197%
15	12.992	1849	1854	1857	rBV	5951803	5446992	82.46%	14.166%
16	13.221	1890	1893	1897	rVB	114557	95492	1.45%	0.248%
17	13.562	1949	1951	1954	rBV	132221	112316	1.70%	0.292%
18	13.892	2000	2007	2017	rBV2	225667	292592	4.43%	0.761%
19	14.039	2028	2032	2036	rBV	1233836	1034434	15.66%	2.690%
20	14.209	2056	2061	2068	rBV	145403	133238	2.02%	0.347%
21	14.515	2109	2113	2117	rVB	127189	112413	1.70%	0.292%
22	14.821	2162	2165	2170	rBV	93578	98223	1.49%	0.255%
23	14.904	2175	2179	2182	rVB	71614	70251	1.06%	0.183%
24	15.168	2220	2224	2230	rBV	81510	97043	1.47%	0.252%
25	15.515	2277	2283	2287	rBV	904988	1133210	17.16%	2.947%
26	15.551	2287	2289	2297	rVB	59830	79704	1.21%	0.207%
27	16.415	2431	2436	2444	rBV8	37531	70818	1.07%	0.184%
28	16.515	2445	2453	2463	rVB5	32845	100193	1.52%	0.261%
29	17.615	2632	2640	2648	rBV7	64997	170052	2.57%	0.442%

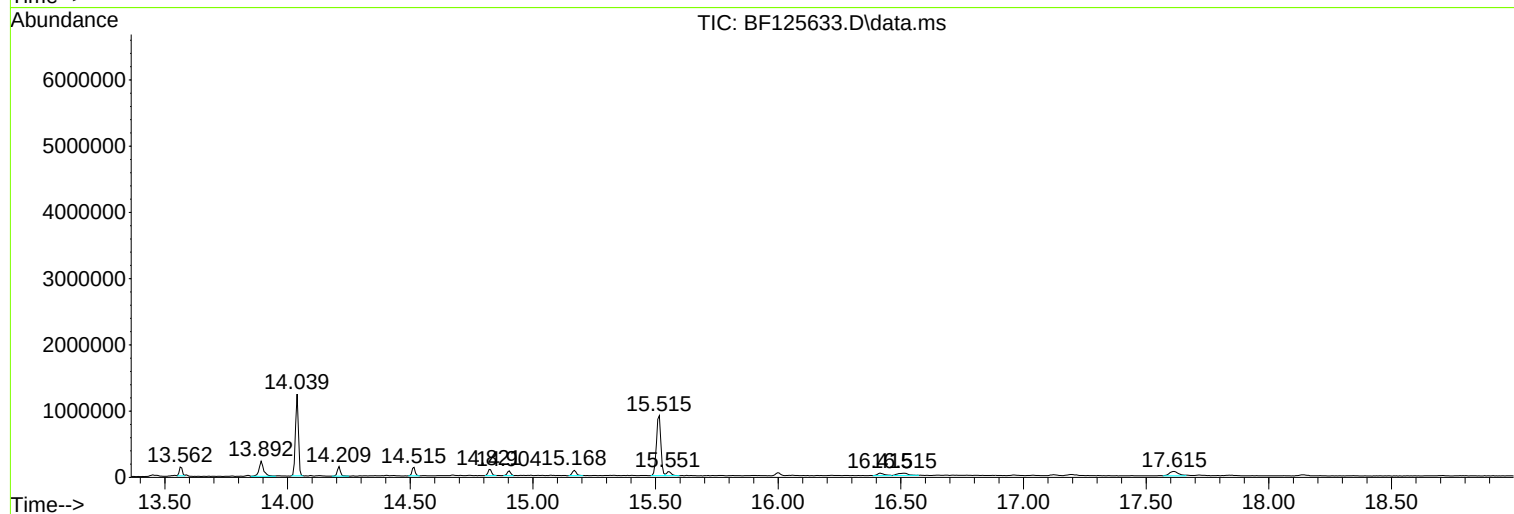
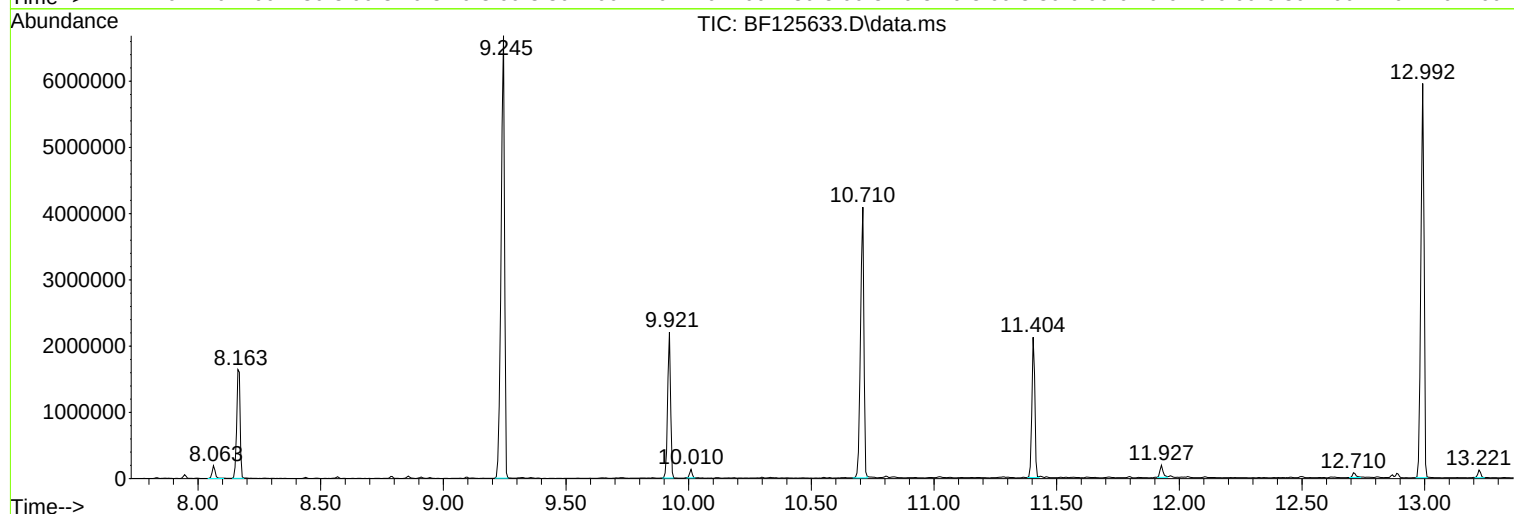
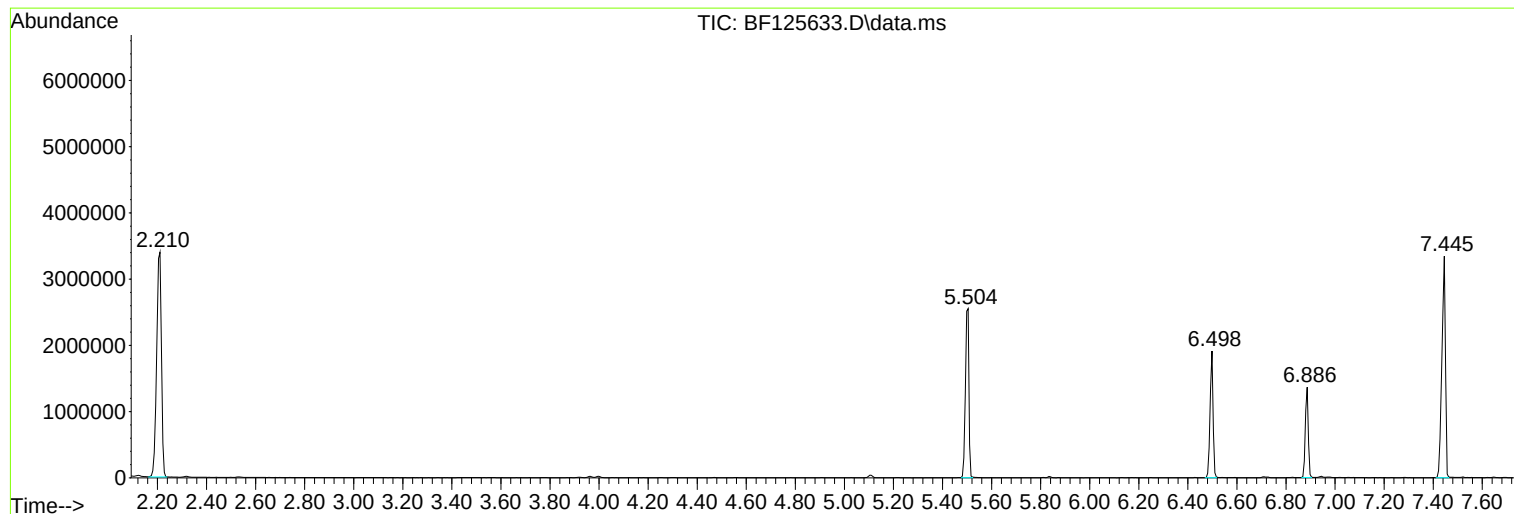
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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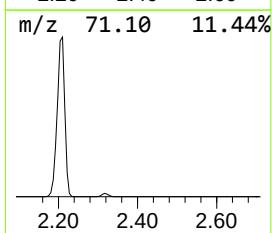
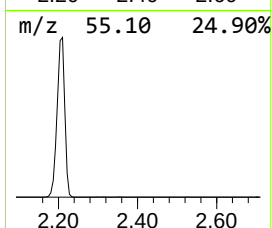
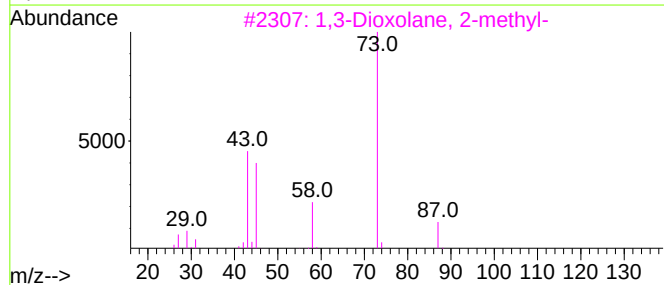
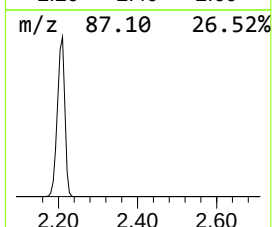
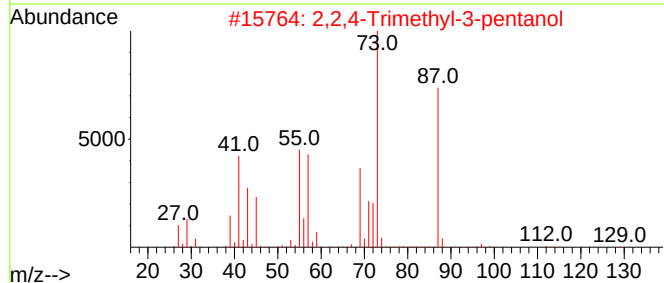
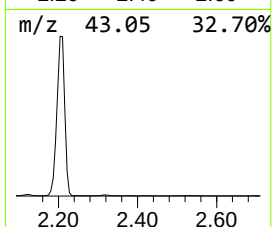
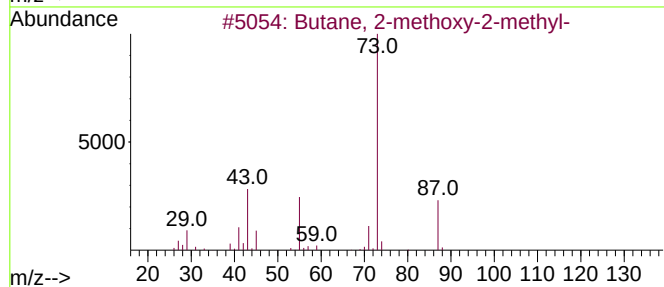
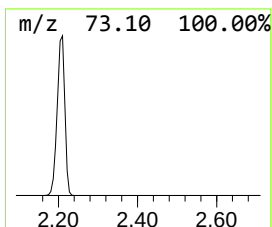
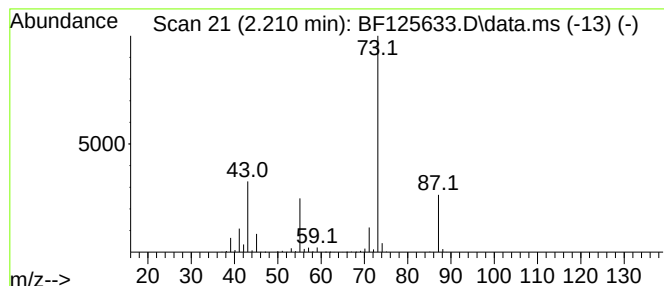
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.210	80.99 ng	4583690	1,4-Dichlorobenzene-d4	6.886

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	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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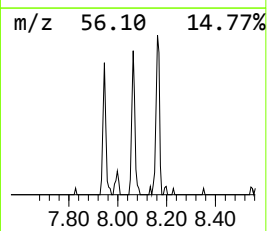
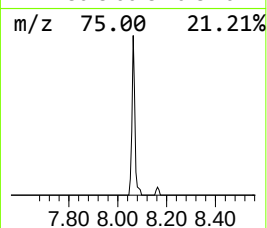
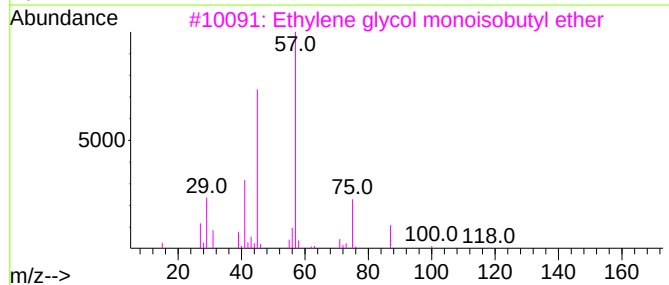
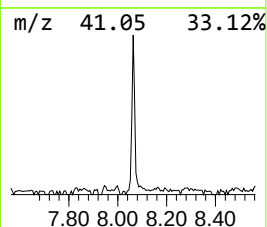
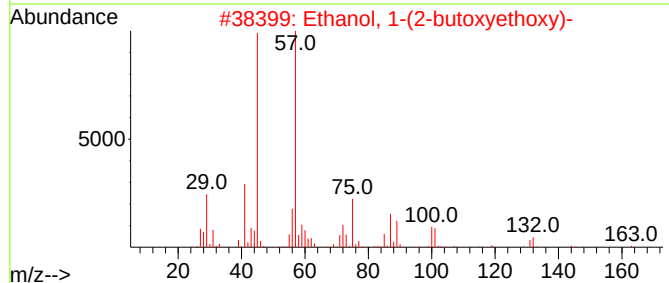
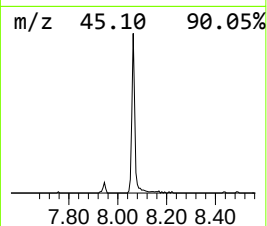
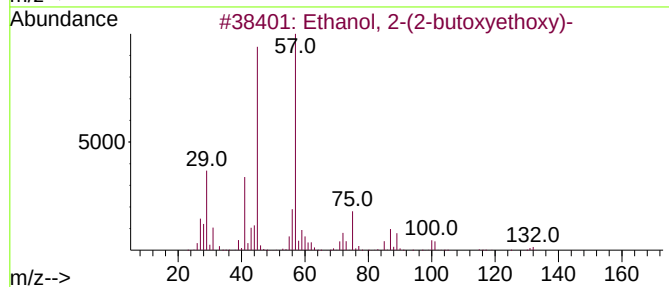
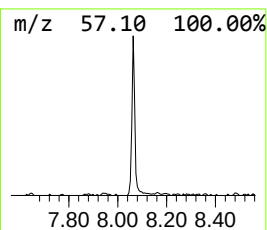
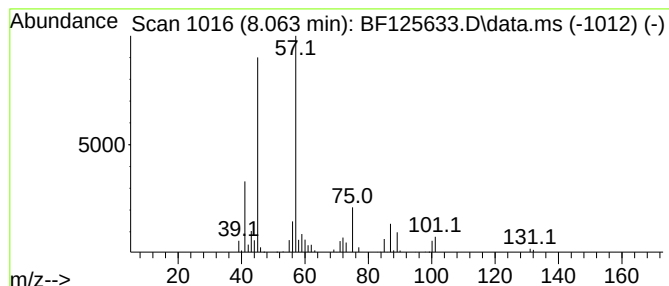
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.063	2.13 ng	169714	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	72
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



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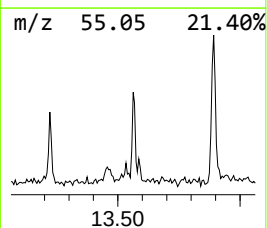
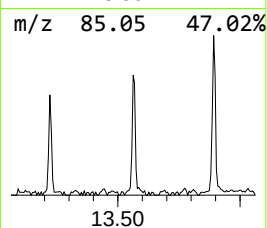
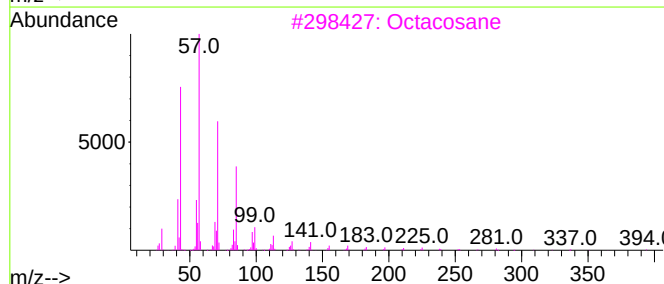
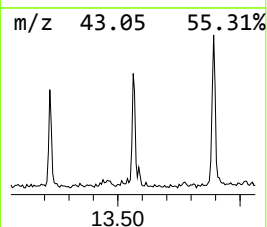
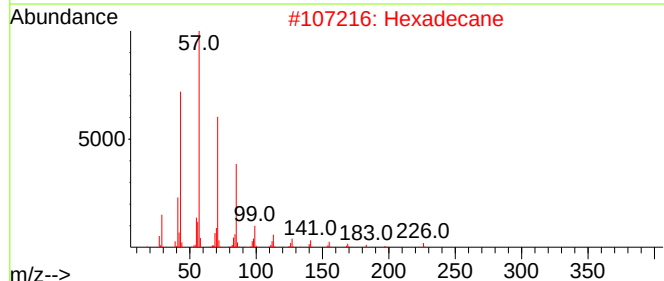
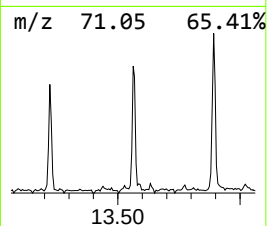
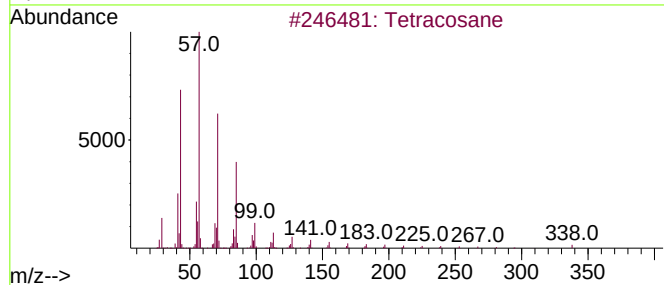
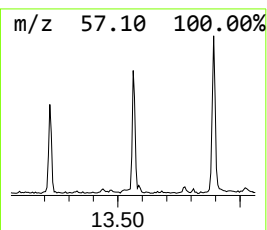
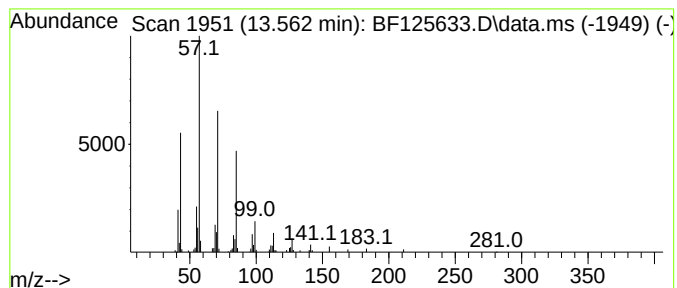
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.562	2.17 ng	112316	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	91
2			Hexadecane	226	C16H34	000544-76-3	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Octadecane	254	C18H38	000593-45-3	90
5			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90



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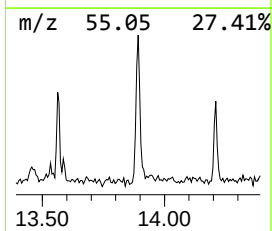
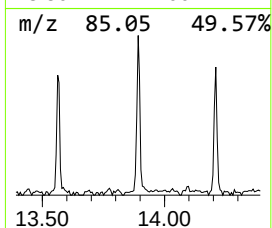
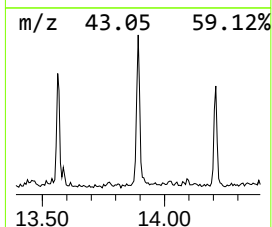
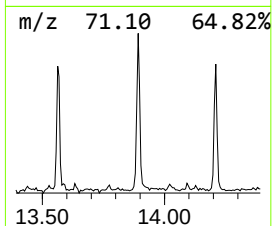
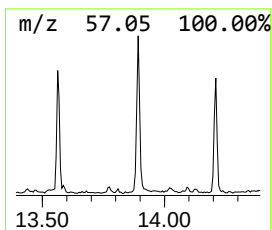
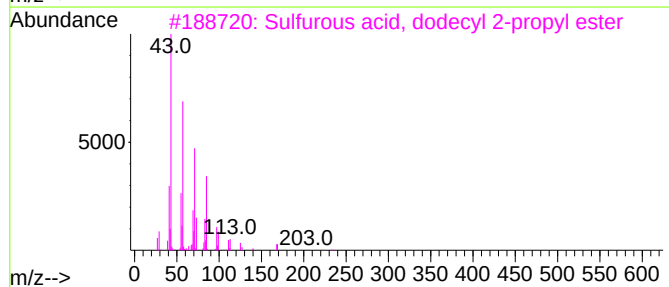
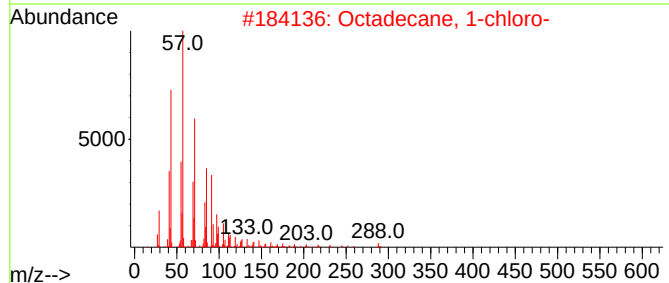
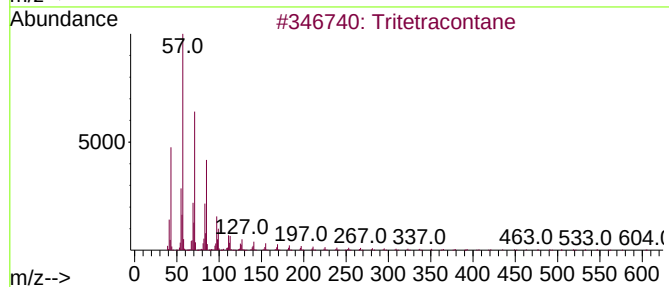
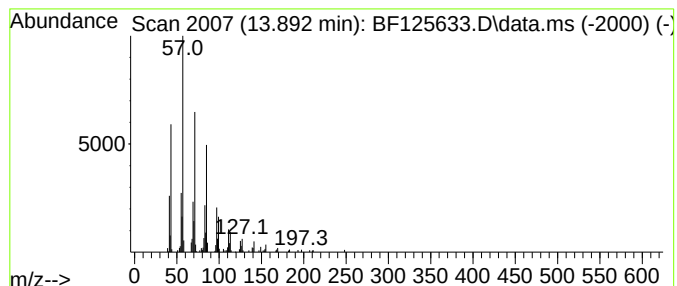
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Tritetracontane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	5.66 ng	292592	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tritetracontane	605	C43H88	007098-21-7	91
2			Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	91
3			Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	91
4			Sulfurous acid, 2-propyl tetradecyl...	320	C17H36O3S	1010309-12-5	91
5			Sulfurous acid, 2-propyl tridecyl...	306	C16H34O3S	1000309-12-4	91



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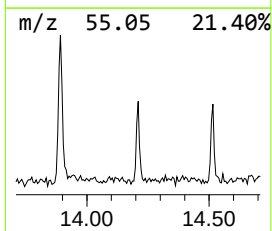
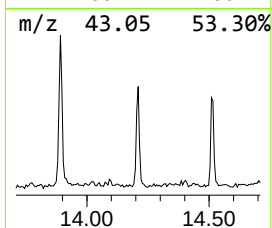
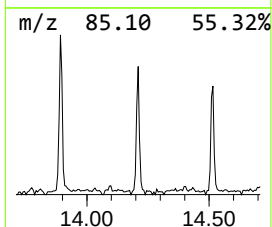
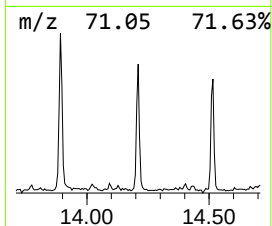
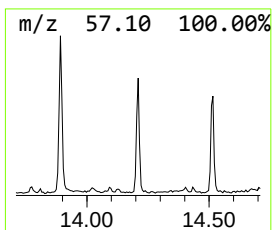
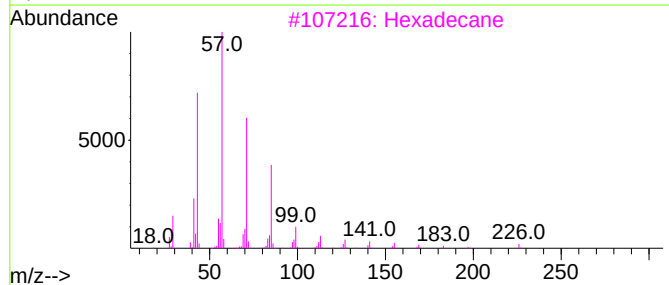
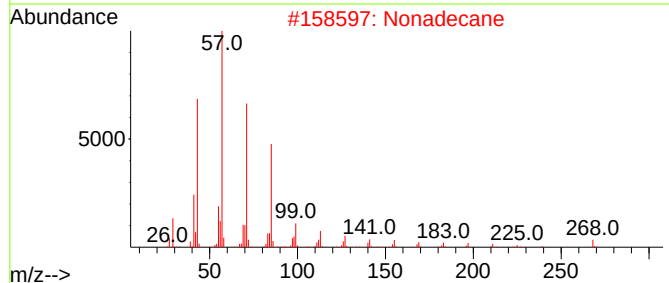
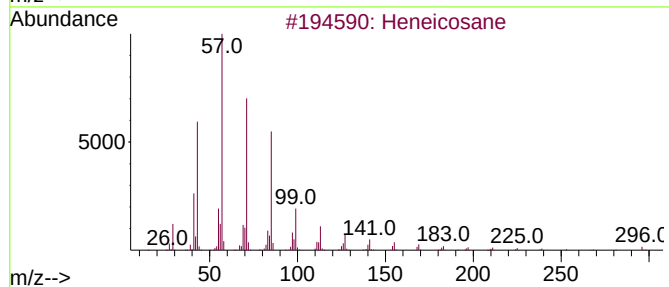
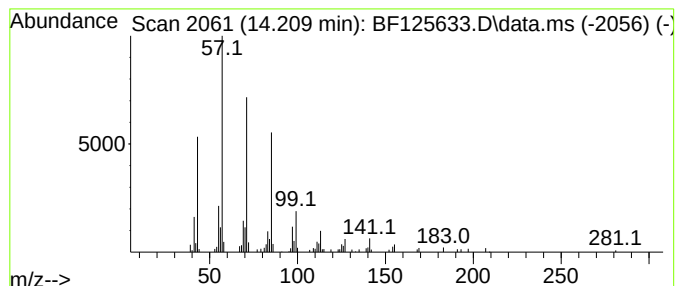
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.209	2.58 ng	133238	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Nonadecane	268	C19H40	000629-92-5	86
3			Hexadecane	226	C16H34	000544-76-3	86
4			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
5			Octadecane	254	C18H38	000593-45-3	86



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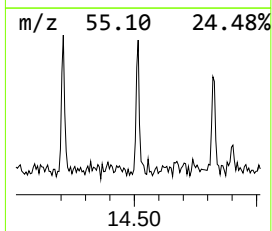
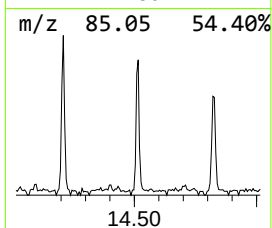
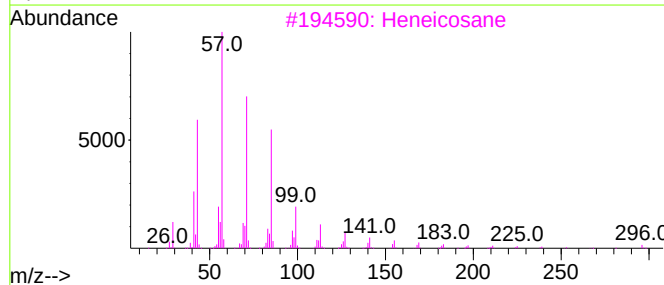
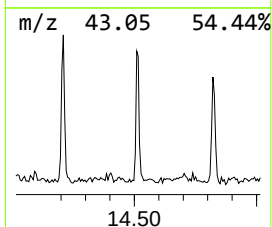
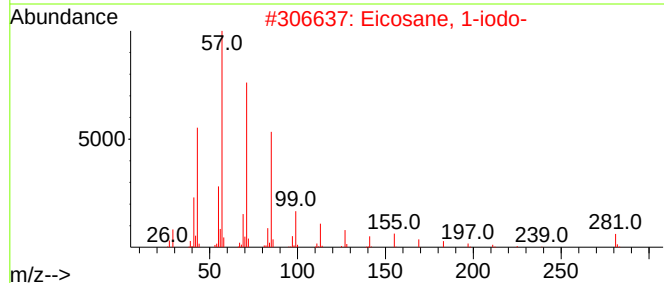
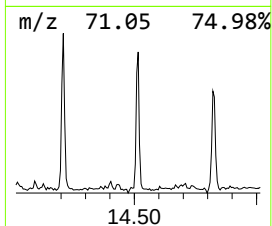
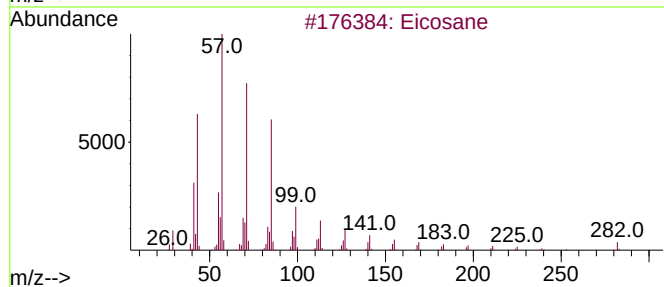
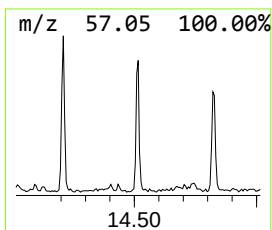
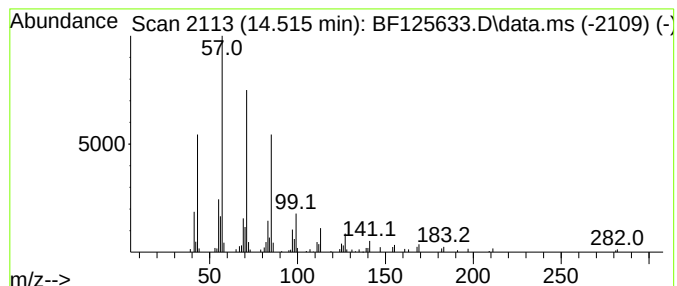
Instrument :
BNA_F
ClientSampleId :
P287-DITCH

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.515	2.17 ng	112413	Chrysene-d12	14.039	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
Data File : BF125633.D
Acq On : 24 Sep 2021 21:52
Operator : JU/CG
Sample : M3911-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P287-DITCH

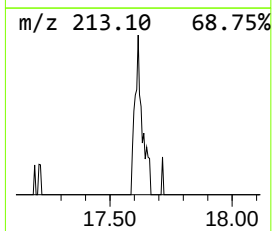
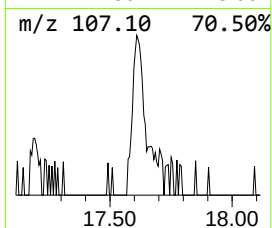
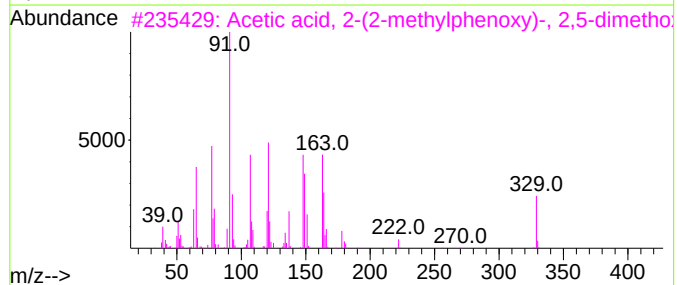
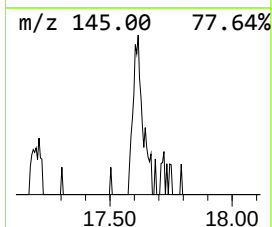
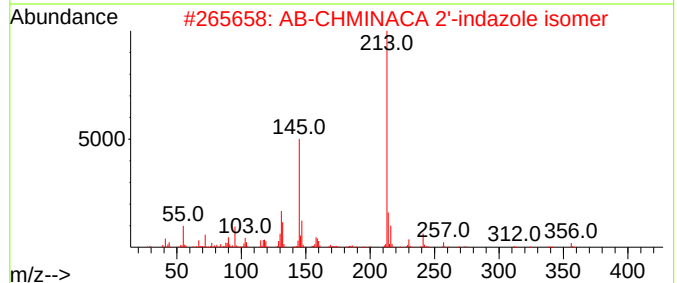
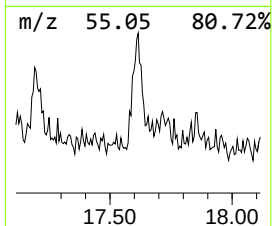
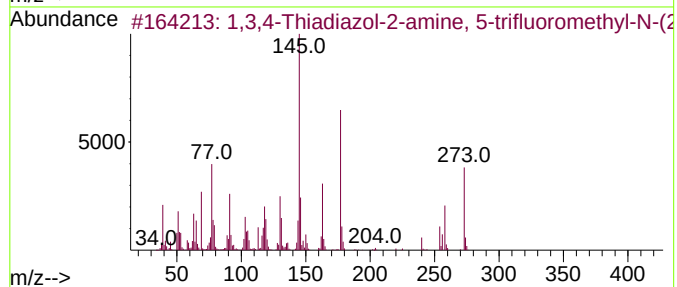
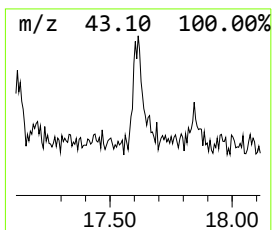
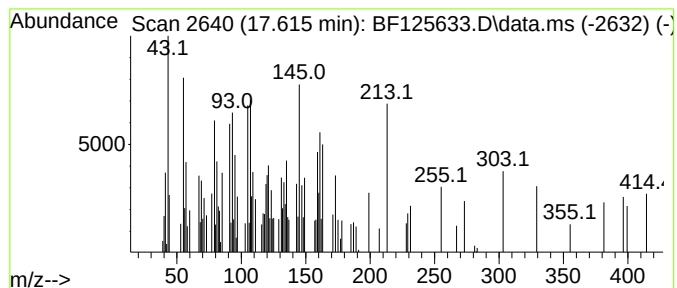
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown17.615 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.615	3.00 ng	170052	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,4-Thiadiazol-2-amine, 5-trif...	273	C11H10F3N3S	284488-18-2	38		
2	AB-CHMINACA 2'-indazole isomer	356	C20H28N4O2	1037296-99-3	16		
3	Acetic acid, 2-(2-methylphenoxy)...	329	C18H19NO5	351061-12-6	15		
4	Cyclopentanecarboxylic acid, 1-p...	273	C14H15N3OS	1000311-03-5	14		
5	Stigmasta-3,5-diene	396	C29H48	004970-37-0	12		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
Data File : BF125633.D
Acq On : 24 Sep 2021 21:52
Operator : JU/CG
Sample : M3911-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P287-DITCH

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.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...	2.210	81.0	ng	4583690	1	6.886	1131870	20.0
Ethanol, 2-(2-b...	8.063	2.1	ng	169714	2	8.169	1594140	20.0
Tetracosane	13.562	2.2	ng	112316	5	14.039	1034430	20.0
Tritetracontane	13.892	5.7	ng	292592	5	14.039	1034430	20.0
Heneicosane	14.209	2.6	ng	133238	5	14.039	1034430	20.0
Eicosane	14.515	2.2	ng	112413	5	14.039	1034430	20.0
unknown17.615	17.615	3.0	ng	170052	6	15.515	1133210	20.0