

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
 Data File : BF127934.D
 Acq On : 27 Apr 2022 01:30
 Operator : CG\JU
 Sample : N2554-01
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RBR-2520253

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-BF042222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127934.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.346	3	10	18	rVB	234060	347147	6.91%	0.958%
2	3.757	219	250	252	rBV	589010	3551219	70.72%	9.803%
3	5.210	493	497	505	rVB	36803	58801	1.17%	0.162%
4	5.581	554	560	563	rBV	4194786	4503754	89.69%	12.433%
5	6.575	722	729	732	rBV	3885048	4668952	92.98%	12.889%
6	6.939	787	791	795	rBV	1097083	883327	17.59%	2.438%
7	7.510	881	888	891	rBV	2975993	3255850	64.84%	8.988%
8	7.669	911	915	919	rVB	71540	63862	1.27%	0.176%
9	8.222	1005	1009	1012	rBV	1178565	1101239	21.93%	3.040%
10	9.304	1187	1193	1196	rBV	5156264	5021278	100.00%	13.861%
11	9.492	1218	1225	1234	rBV4	21850	61950	1.23%	0.171%
12	9.980	1302	1308	1311	rBV	1330996	1216476	24.23%	3.358%
13	10.016	1311	1314	1317	rVB	168066	136985	2.73%	0.378%
14	10.186	1337	1343	1346	rBV	52950	53611	1.07%	0.148%
15	10.774	1439	1443	1447	rBV	2945949	2860740	56.97%	7.897%
16	10.898	1461	1464	1470	rVB3	41011	51698	1.03%	0.143%
17	10.951	1470	1473	1475	rBV	78576	74650	1.49%	0.206%
18	10.980	1475	1478	1482	rVB3	61068	74867	1.49%	0.207%
19	11.016	1482	1484	1487	rBV	58803	50558	1.01%	0.140%
20	11.127	1500	1503	1507	rVB2	65236	75552	1.50%	0.209%
21	11.169	1507	1510	1513	rBV	73658	71554	1.43%	0.198%
22	11.474	1558	1562	1564	rBV	1215977	999247	19.90%	2.758%
23	11.498	1564	1566	1570	rVB	231348	177298	3.53%	0.489%
24	11.986	1645	1649	1655	rBV3	166724	212005	4.22%	0.585%
25	12.692	1765	1769	1772	rBV	295598	273081	5.44%	0.754%
26	12.921	1802	1808	1811	rBV	259631	263415	5.25%	0.727%
27	12.951	1811	1813	1820	rVB2	37645	66582	1.33%	0.184%
28	13.063	1828	1832	1835	rBV	3728395	3370214	67.12%	9.304%
29	13.998	1986	1991	2000	rBV3	160690	310778	6.19%	0.858%
30	14.086	2003	2006	2008	rVV	254498	225643	4.49%	0.623%
31	14.121	2008	2012	2015	rVV	923975	954717	19.01%	2.636%
32	14.145	2015	2016	2023	rVB	147781	109962	2.19%	0.304%
33	15.186	2190	2193	2197	rBV	113715	181733	3.62%	0.502%
34	15.245	2200	2203	2209	rVB	109223	129255	2.57%	0.357%
35	15.568	2256	2258	2263	rVV	59200	61963	1.23%	0.171%
36	15.639	2265	2270	2281	rVB	516923	705215	14.04%	1.947%

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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-BF042222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

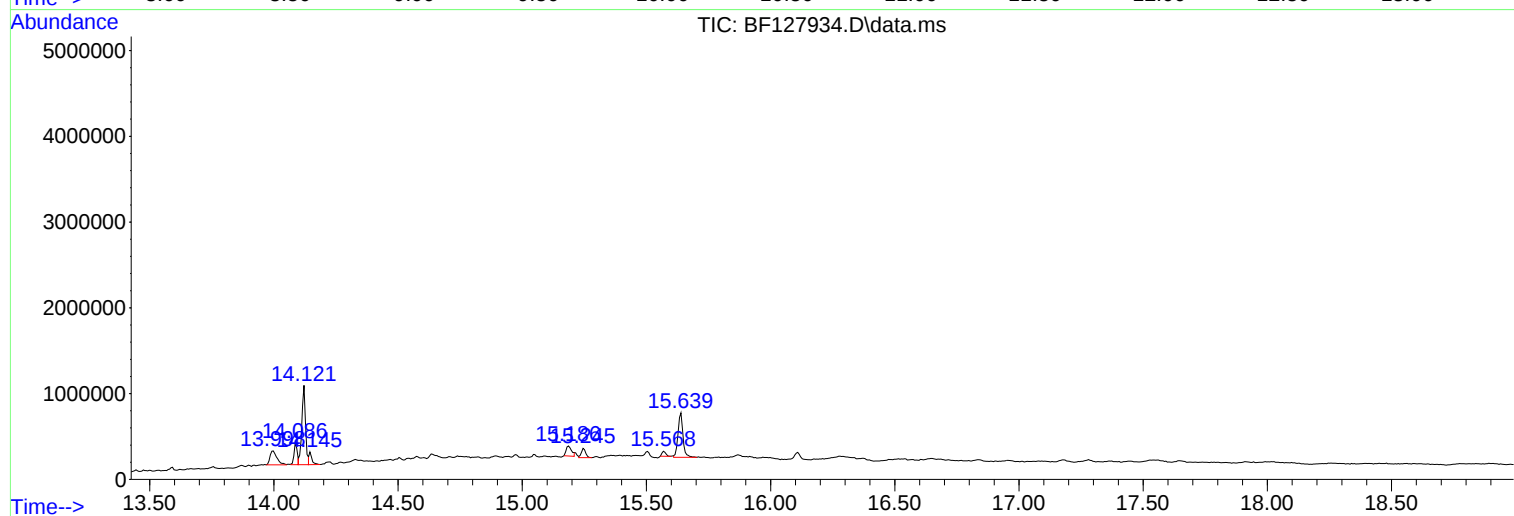
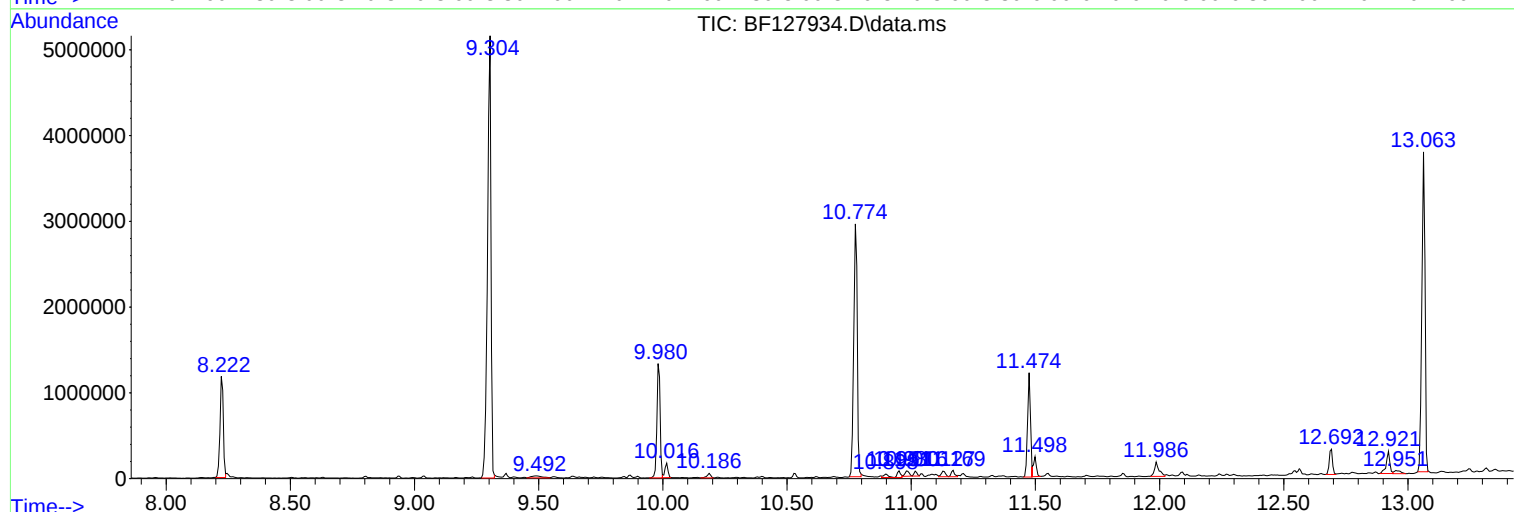
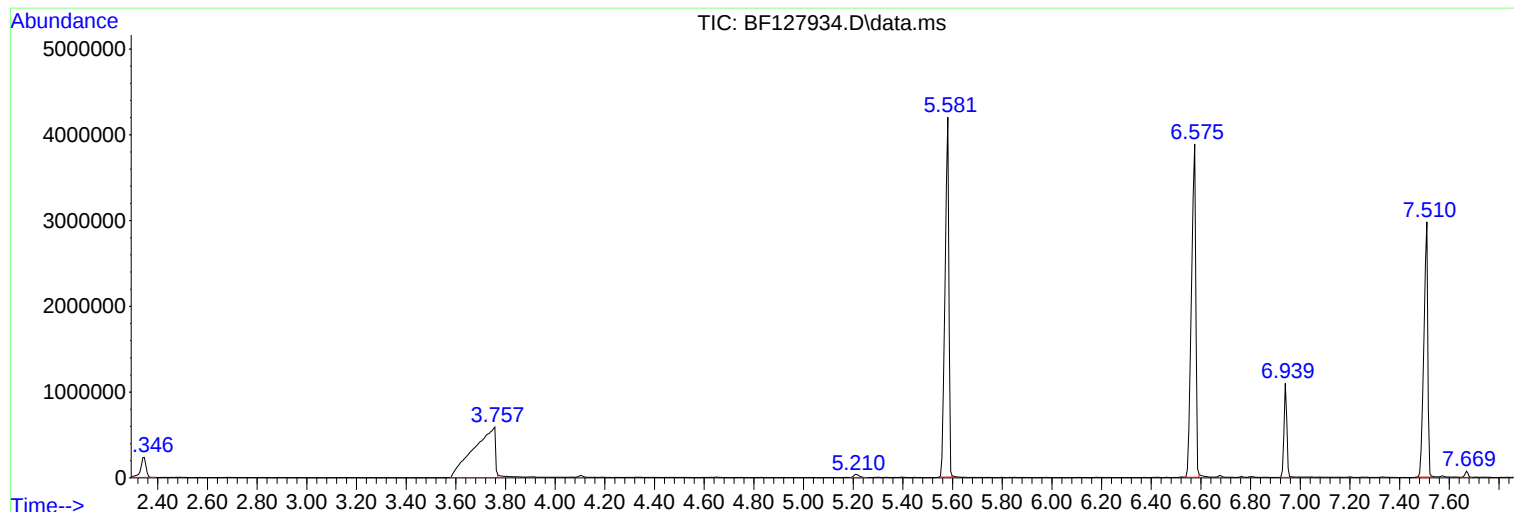
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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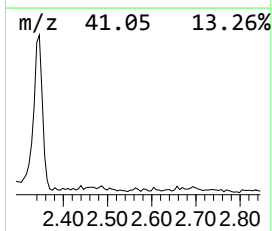
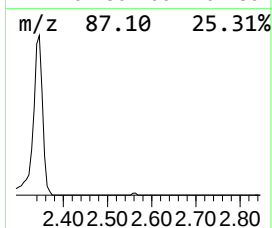
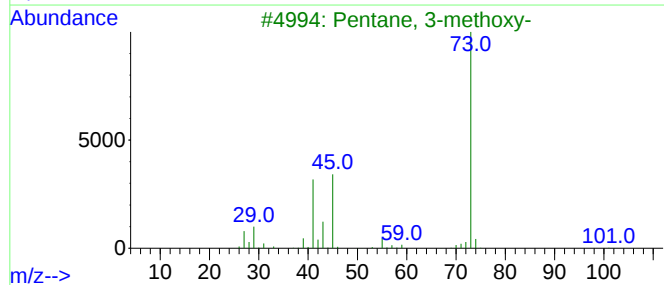
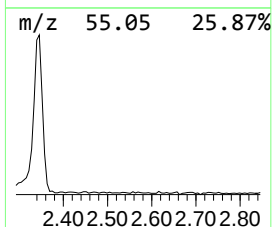
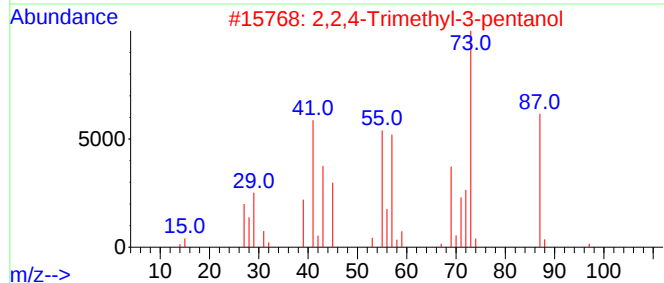
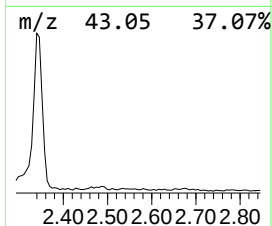
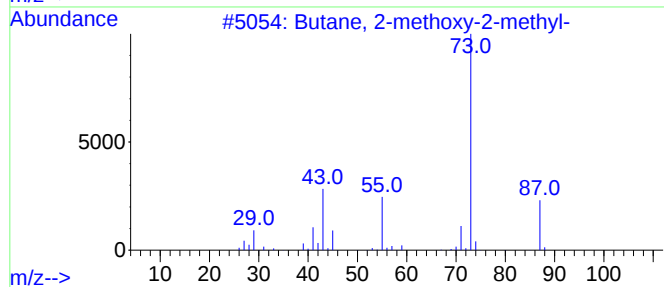
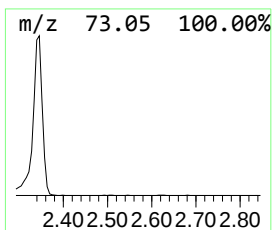
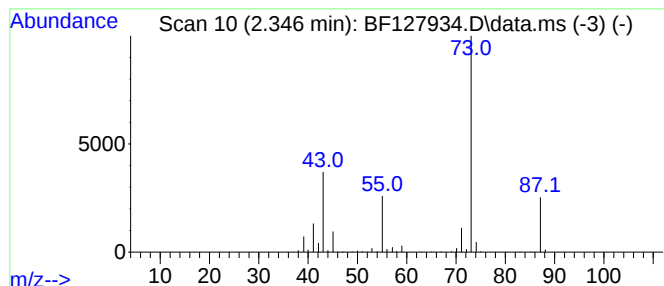
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.346	7.86 ng	347147	1,4-Dichlorobenzene-d4	6.939

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	56
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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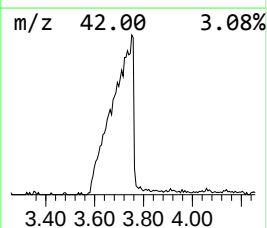
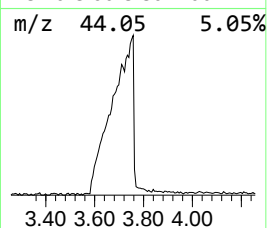
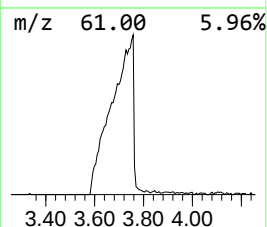
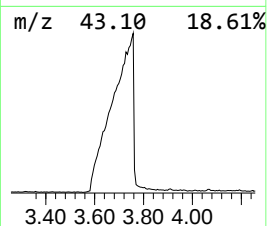
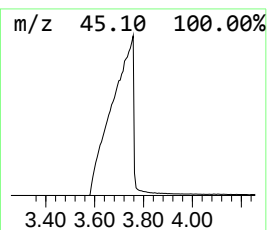
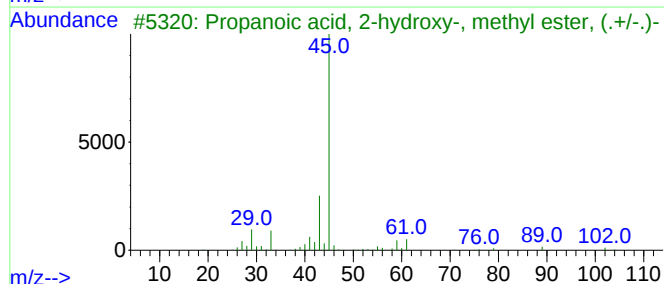
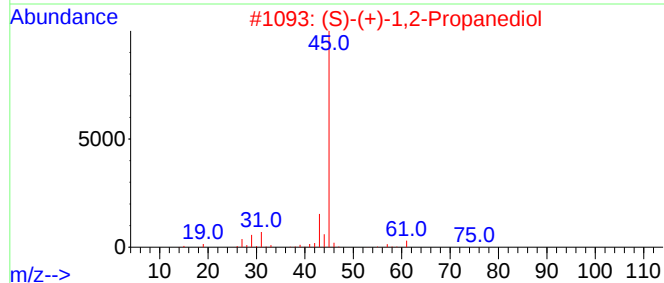
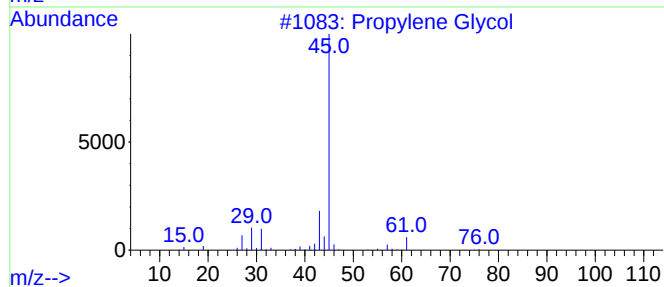
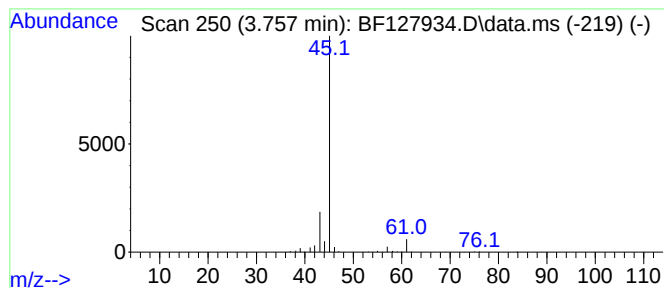
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Propylene Glycol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.757	80.41 ng	3551220	1,4-Dichlorobenzene-d4	6.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	90
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	9
5			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9



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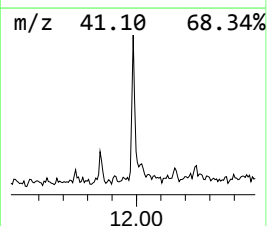
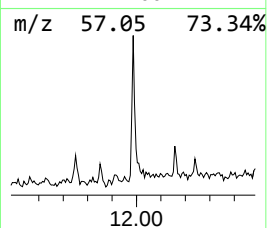
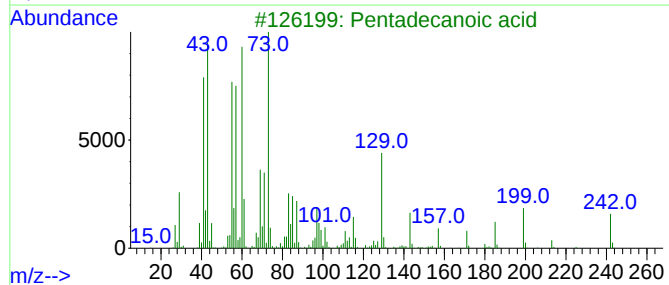
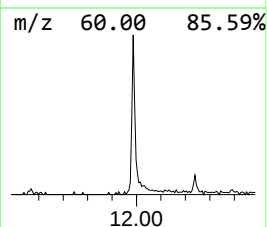
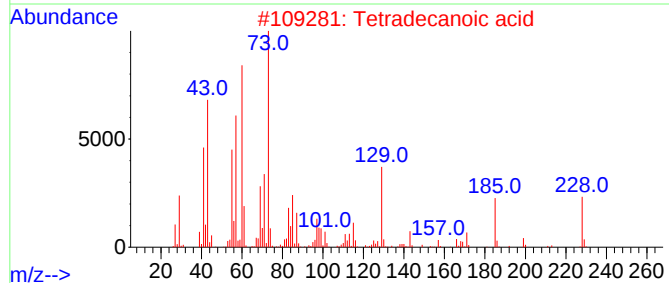
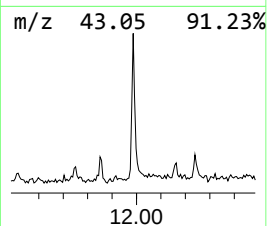
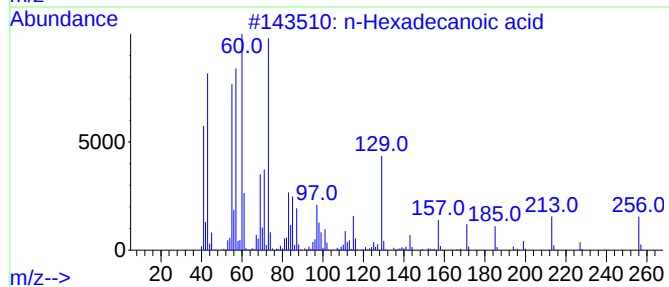
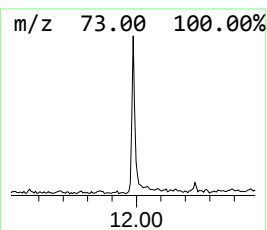
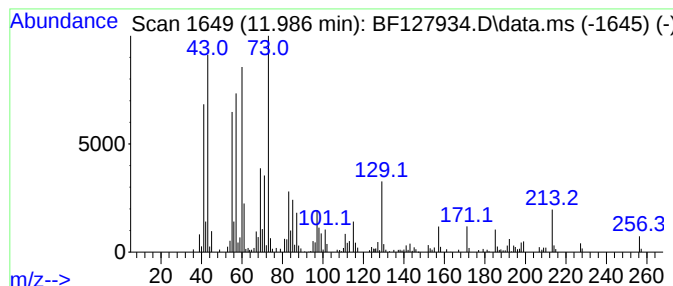
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.986	4.24 ng	212005	Phenanthrene-d10	11.474

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	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	81
5			Isopropyl palmitate	298	C19H38O2	000142-91-6	64



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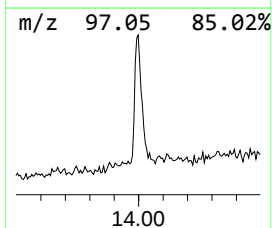
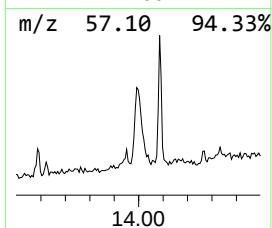
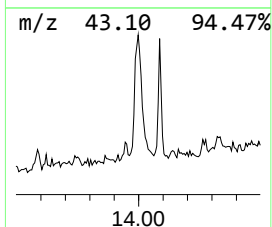
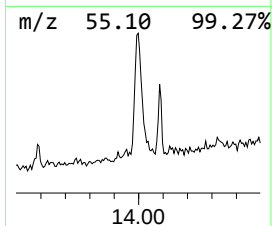
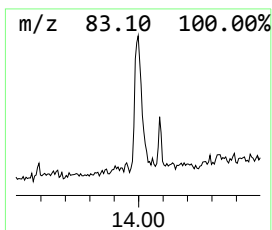
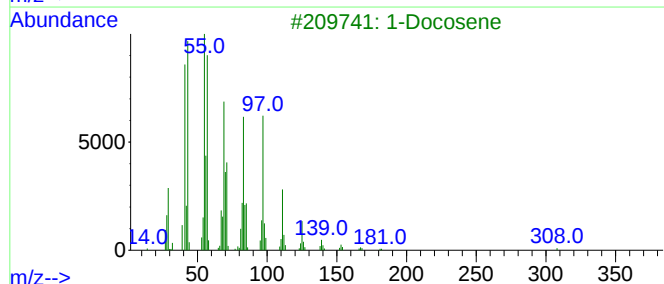
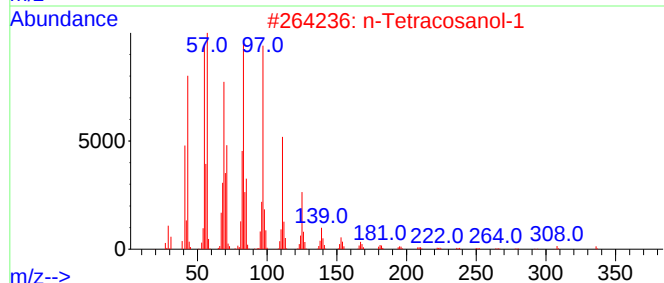
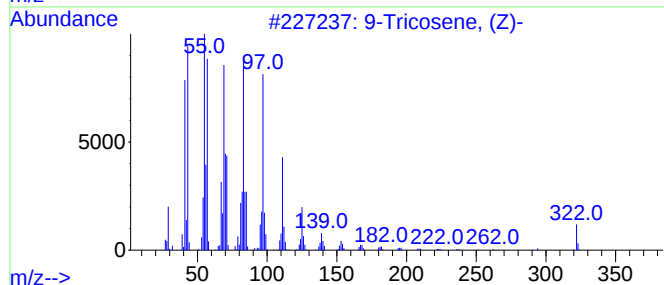
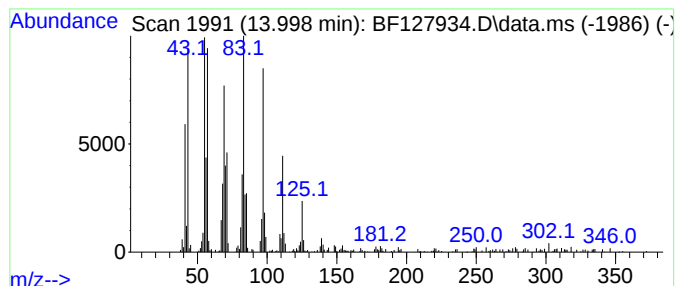
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Tricosene, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	6.51 ng	310778	Chrysene-d12	14.121

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Tricosene, (Z)-	322	C23H46	027519-02-4	94
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3		1-Docosene	308	C22H44	001599-67-3	93
4		Behenic alcohol	326	C22H46O	000661-19-8	91
5		Pentacos-1-ene	350	C25H50	016980-85-1	91



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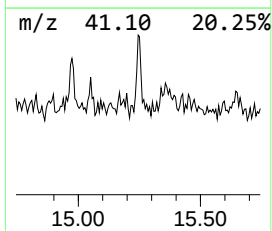
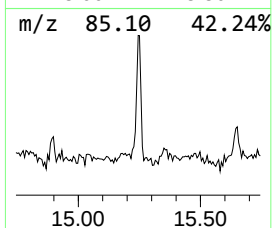
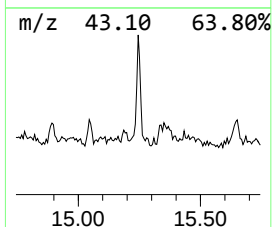
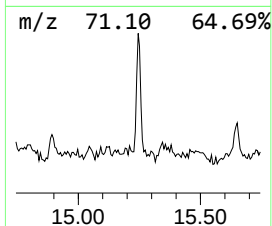
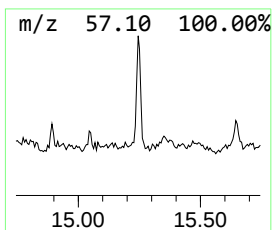
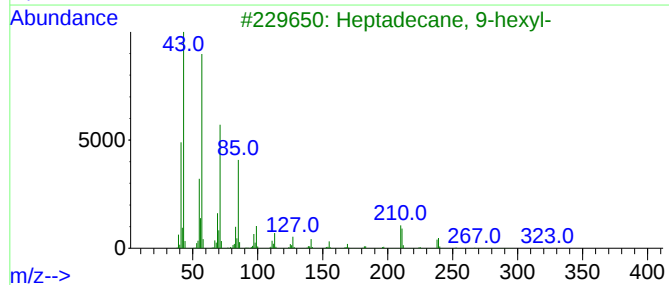
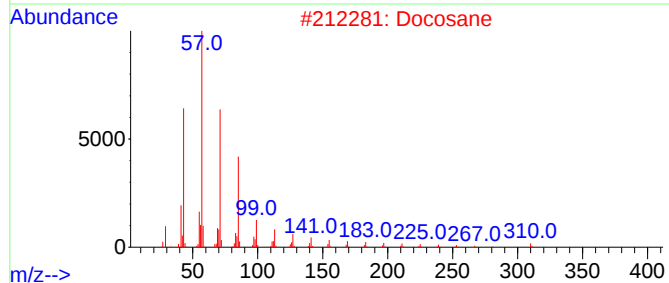
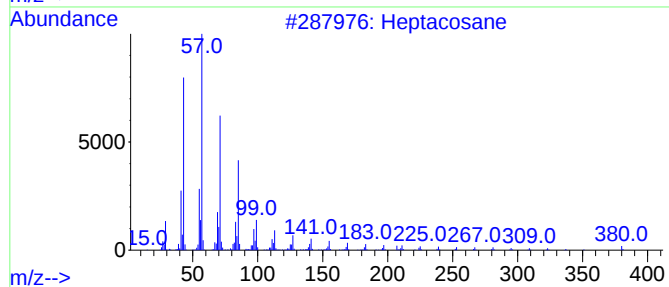
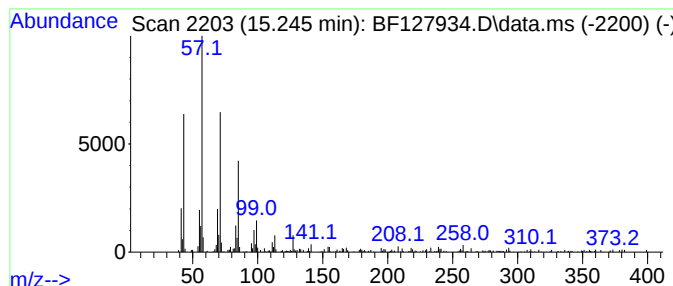
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.245	3.67 ng	129255	Perylene-d12	15.639

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	95
2			Docosane	310	C22H46	000629-97-0	93
3			Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	93
4			Tetracosane	338	C24H50	000646-31-1	93
5			Heptadecane	240	C17H36	000629-78-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
Data File : BF127934.D
Acq On : 27 Apr 2022 01:30
Operator : CG\JU
Sample : N2554-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-2520253

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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...	2.346	7.9	ng	347147	1	6.939	883327	20.0
Propylene Glycol	3.757	80.4	ng	3551220	1	6.939	883327	20.0
n-Hexadecanoic ...	11.986	4.2	ng	212005	4	11.474	999247	20.0
9-Tricosene, (Z)-	13.998	6.5	ng	310778	5	14.121	954717	20.0
Heptacosane	15.245	3.7	ng	129255	6	15.639	705215	20.0