

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030124\
 Data File : BF137455.D
 Acq On : 01 Mar 2024 13:18
 Operator : CG\JU
 Sample : P1653-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 294

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-BF022924.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137455.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	5	11	22	rVB	1071453	1429015	38.31%	5.017%
2	3.499	237	240	255	rBV	59356	176520	4.73%	0.620%
3	5.128	514	517	522	rBV	35788	39874	1.07%	0.140%
4	5.516	579	583	606	rBV	3563608	3433345	92.05%	12.053%
5	6.504	747	751	773	rBV	3605803	3466921	92.96%	12.170%
6	6.863	809	812	822	rBV	1053478	1030832	27.64%	3.619%
7	7.422	904	907	920	rBV	2148829	2058352	55.19%	7.226%
8	8.140	1025	1029	1047	rBV	1578233	1380872	37.02%	4.847%
9	8.463	1081	1084	1098	rBV	45434	78510	2.11%	0.276%
10	9.216	1209	1212	1225	rBV	3980923	3729671	100.00%	13.093%
11	9.898	1324	1328	1332	rBV	1718955	1418387	38.03%	4.979%
12	10.004	1341	1346	1359	rBV	681911	949322	25.45%	3.333%
13	10.692	1459	1463	1480	rBV	1721263	1769245	47.44%	6.211%
14	11.392	1578	1582	1585	rBV	1428479	1225396	32.86%	4.302%
15	11.416	1585	1586	1592	rVB	114307	88438	2.37%	0.310%
16	11.939	1671	1675	1684	rBV3	131900	202085	5.42%	0.709%
17	12.610	1786	1789	1796	rBV	157486	161878	4.34%	0.568%
18	12.727	1805	1809	1814	rBV5	32300	48122	1.29%	0.169%
19	12.839	1823	1828	1833	rBV	143045	166074	4.45%	0.583%
20	12.992	1850	1854	1863	rBV	3262519	2788374	74.76%	9.788%
21	13.175	1879	1885	1890	rVB3	21985	41924	1.12%	0.147%
22	13.916	2007	2011	2023	rBV	106611	183790	4.93%	0.645%
23	14.051	2029	2034	2038	rBV	1212446	1180733	31.66%	4.145%
24	14.545	2114	2118	2121	rBV3	35911	41285	1.11%	0.145%
25	14.951	2183	2187	2192	rBV	50285	65869	1.77%	0.231%
26	15.127	2213	2217	2220	rBV	56480	88583	2.38%	0.311%
27	15.239	2233	2236	2241	rVB3	33775	44303	1.19%	0.156%
28	15.451	2267	2272	2279	rVB2	33641	58041	1.56%	0.204%
29	15.516	2279	2283	2289	rBV	37544	59679	1.60%	0.210%
30	15.580	2289	2294	2305	rBV	697062	977074	26.20%	3.430%
31	16.139	2385	2389	2395	rBV2	23356	43554	1.17%	0.153%
32	16.204	2395	2400	2408	rVV7	27835	60205	1.61%	0.211%

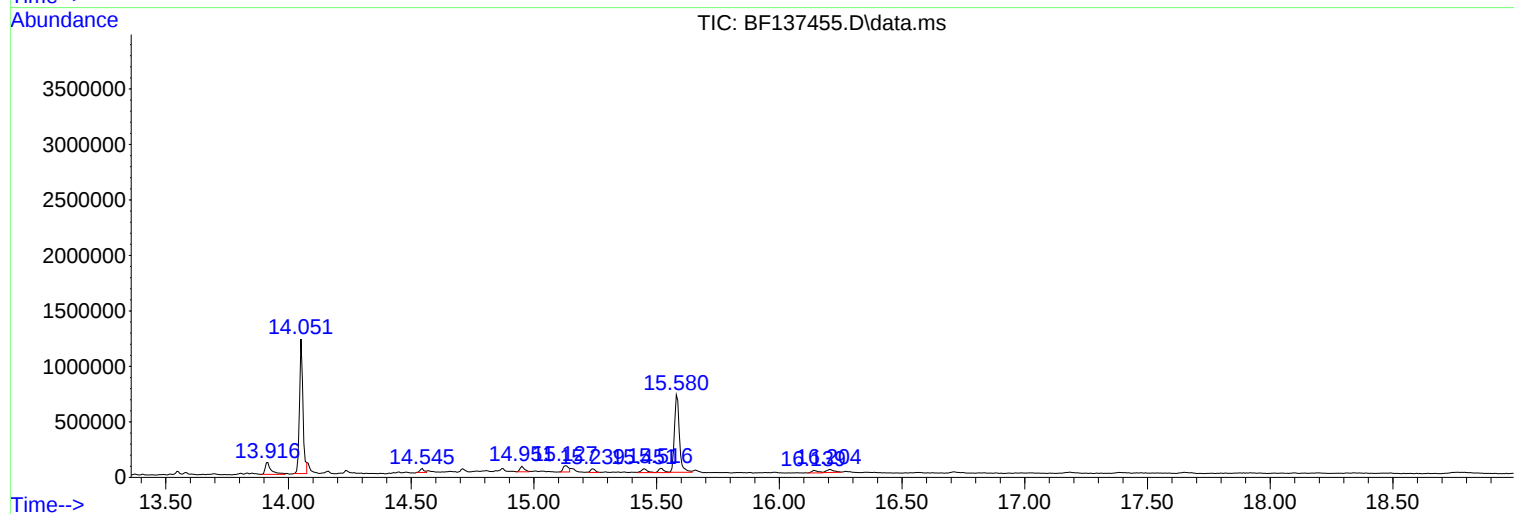
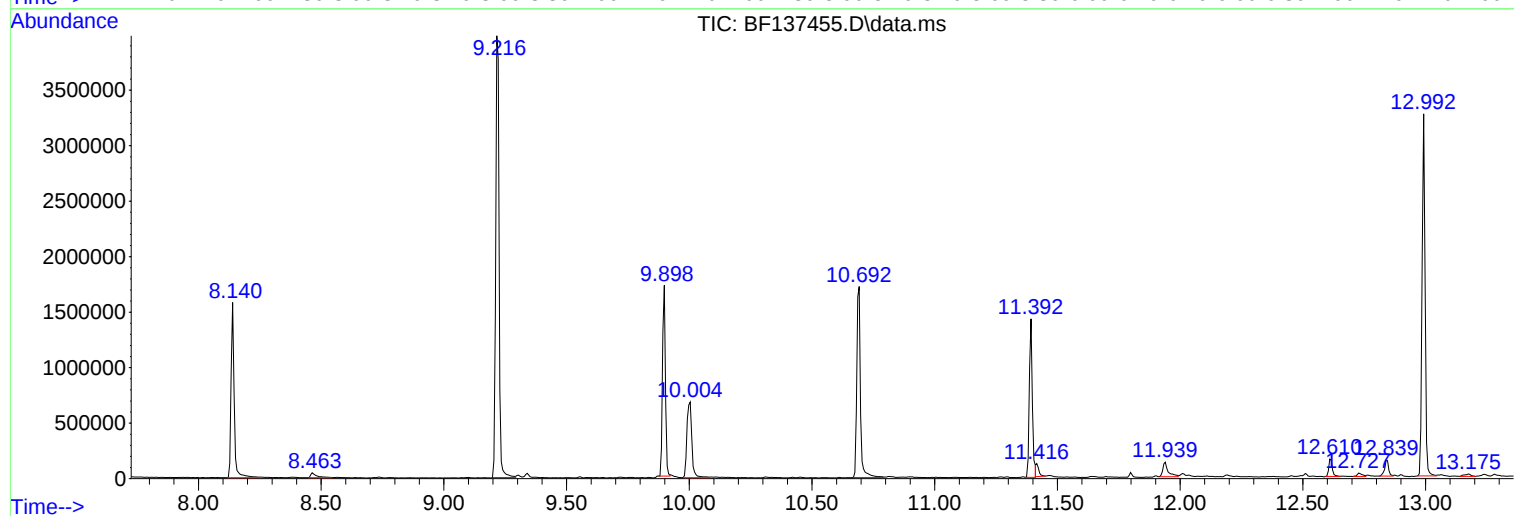
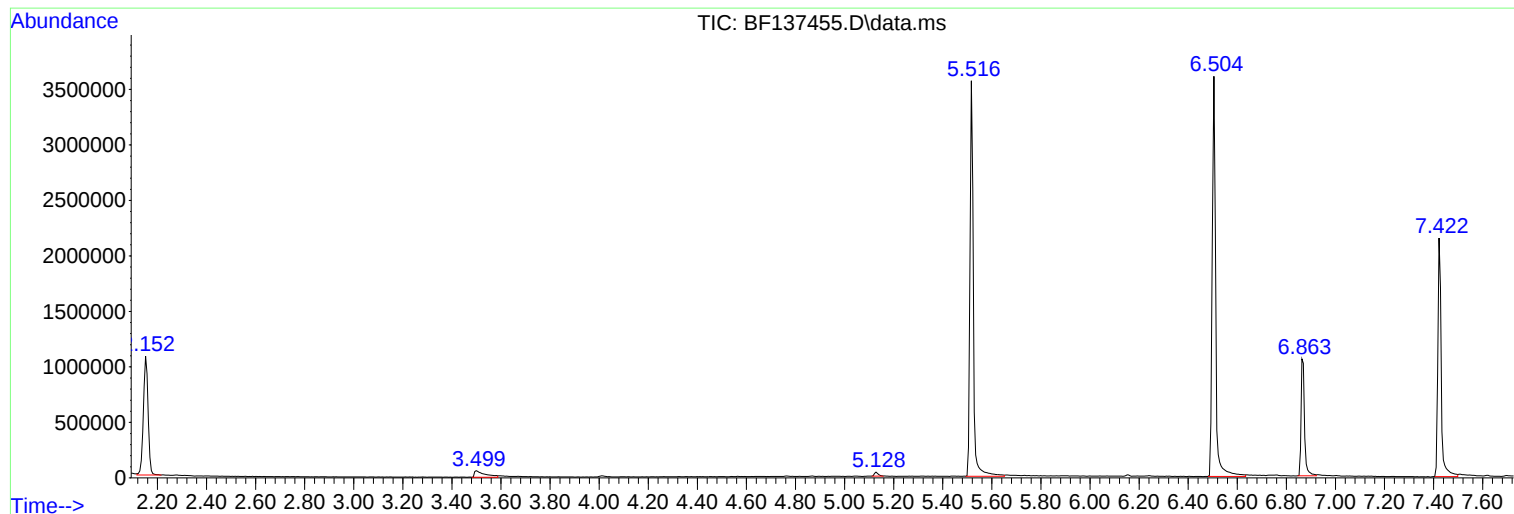
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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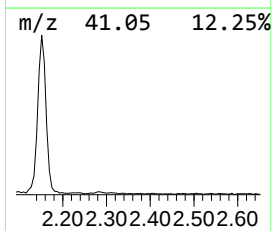
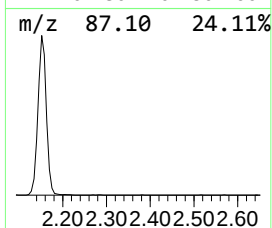
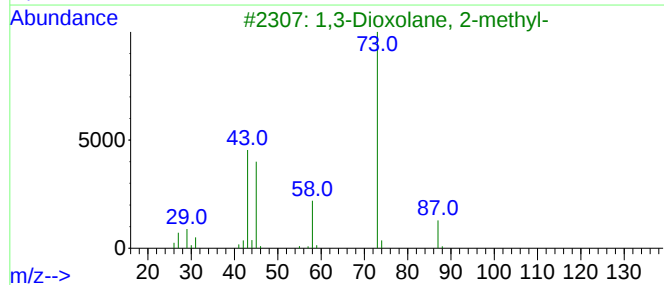
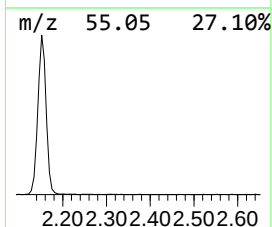
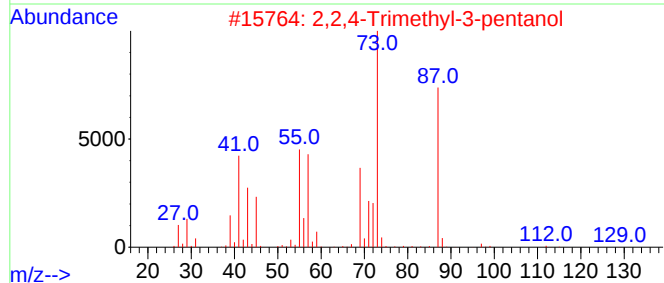
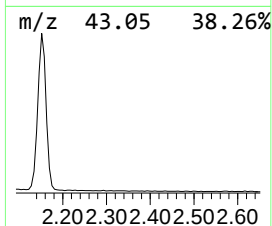
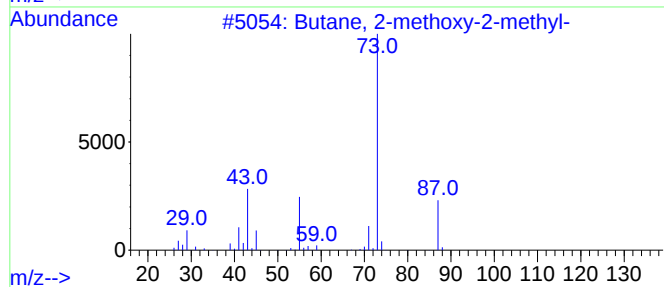
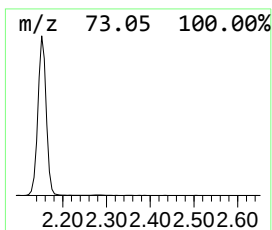
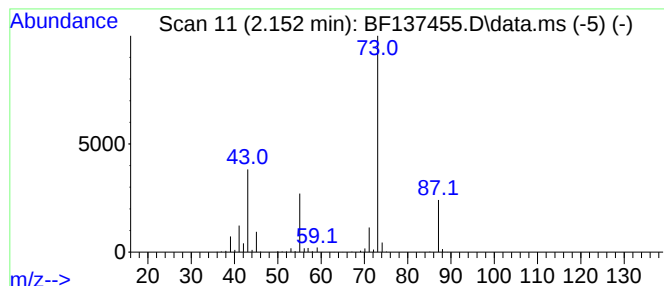
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.152	27.73 ng	1429020	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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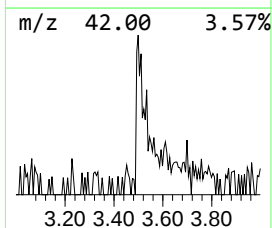
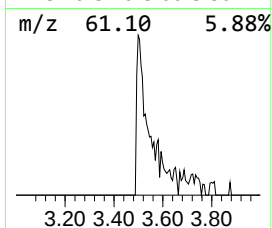
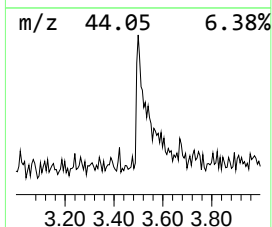
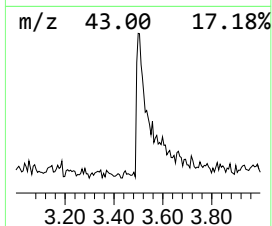
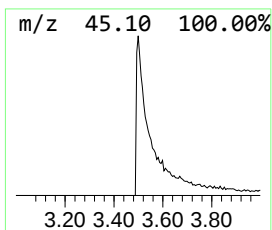
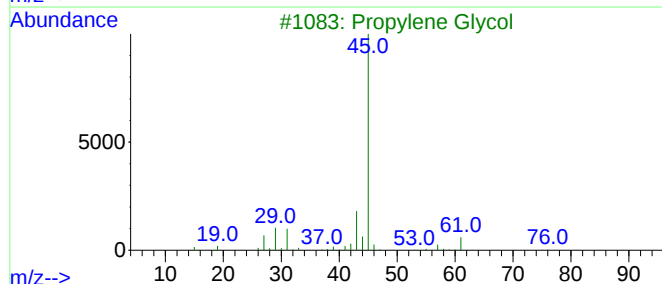
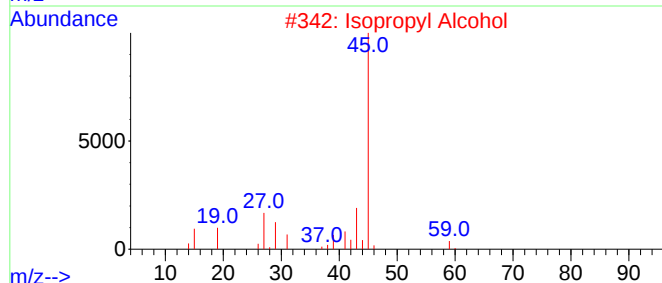
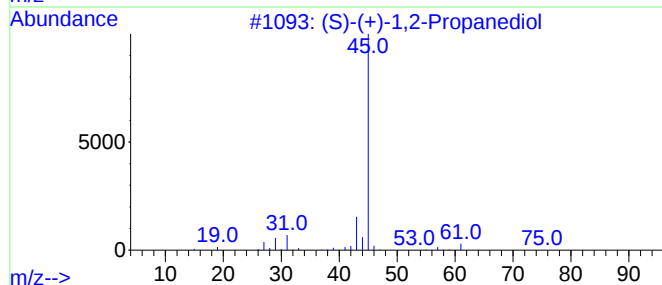
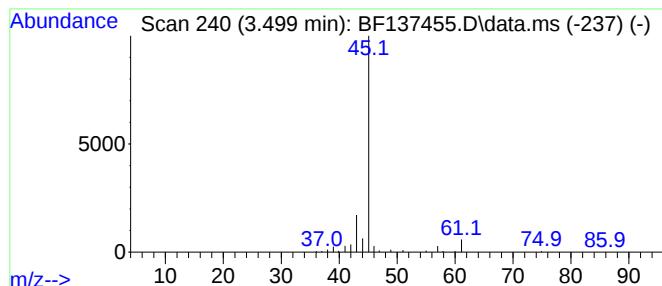
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.499	3.42 ng	176520	1,4-Dichlorobenzene-d4	6.869

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2		Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3		Propylene Glycol	76	C3H8O2	000057-55-6	43
4		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
5		2-Butanol	74	C4H10O	000078-92-2	40



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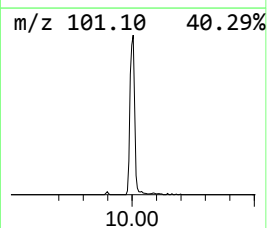
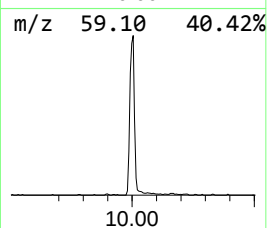
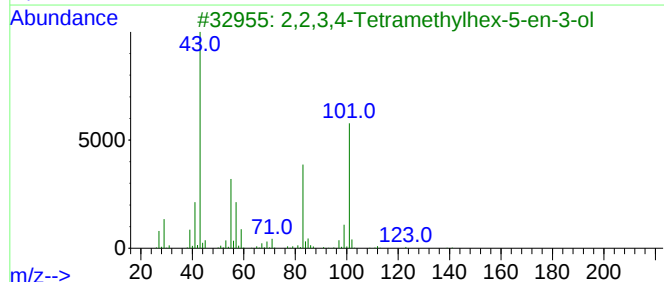
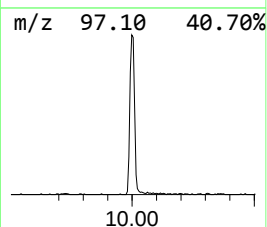
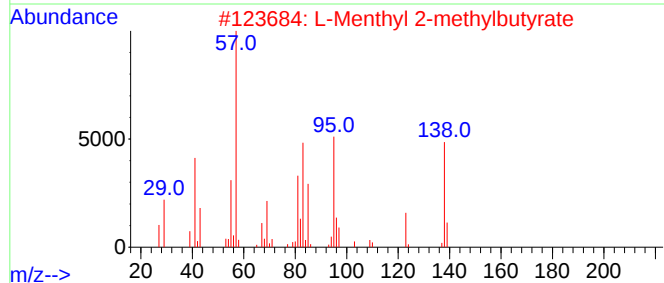
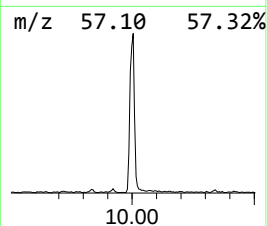
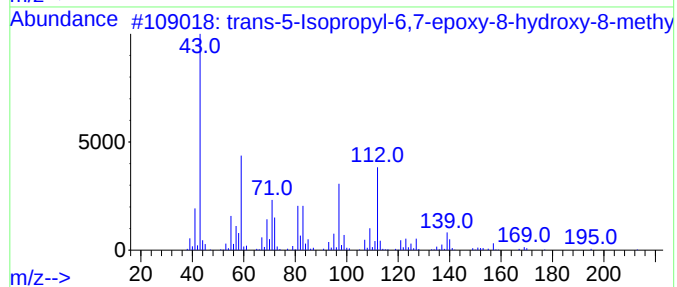
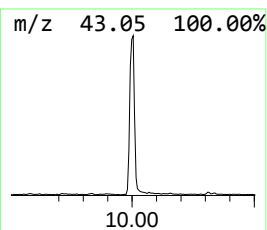
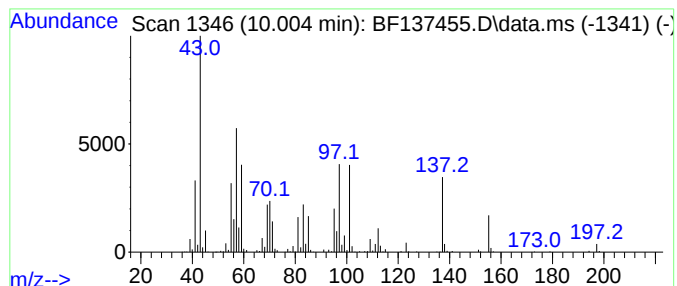
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Peak Number 3 unknown10.004 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.004	13.39 ng	949322	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	16
2			L-Menthyl 2-methylbutyrate	240	C15H28O2	1000429-43-8	14
3			2,2,3,4-Tetramethylhex-5-en-3-ol	156	C10H20O	1010191-06-9	14
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	12
5			Carbonic acid, octyl prop-1-en-2...	214	C12H22O3	1000382-54-0	12



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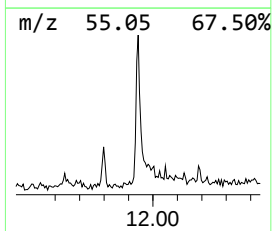
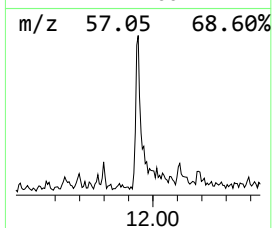
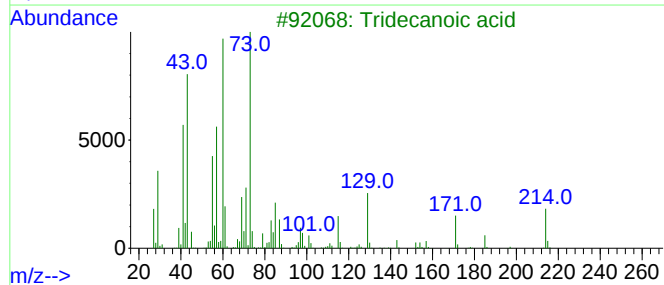
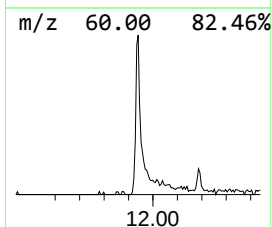
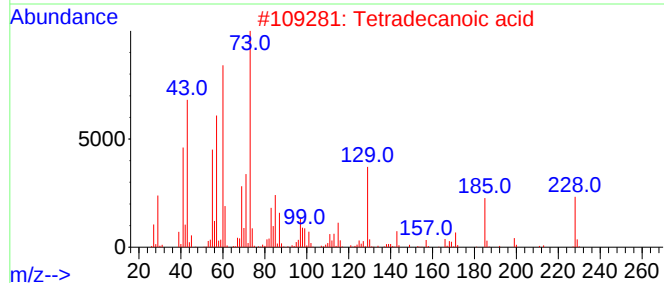
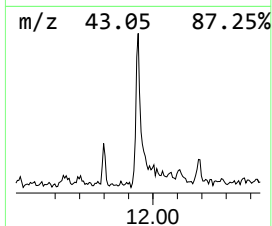
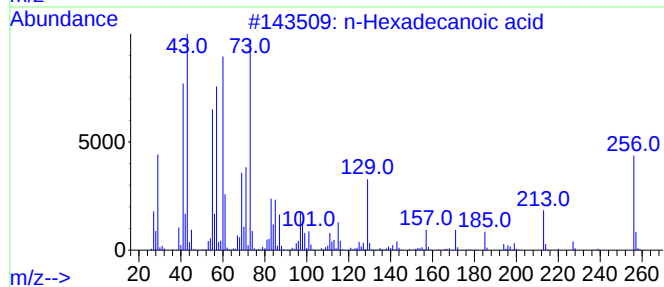
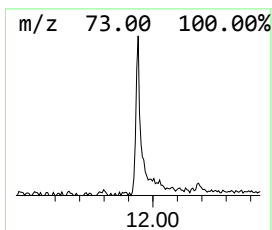
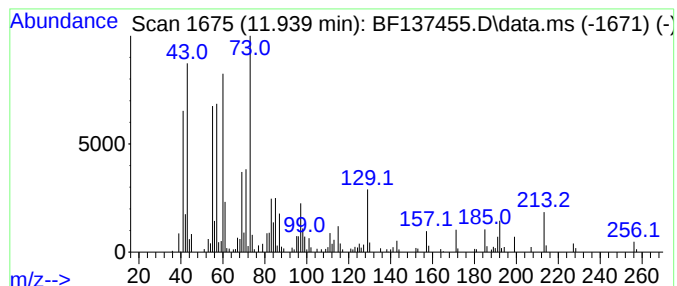
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	3.30 ng	202085	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3			Tridecanoic acid	214	C13H26O2	000638-53-9	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5			Nonanoic acid	158	C9H18O2	000112-05-0	50



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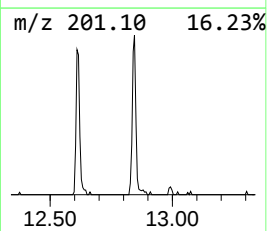
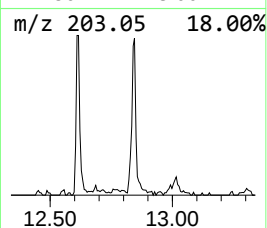
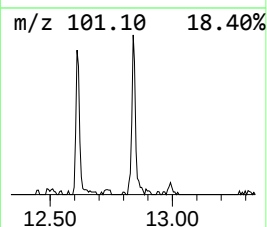
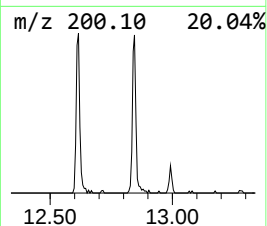
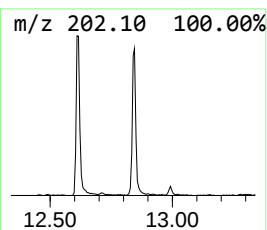
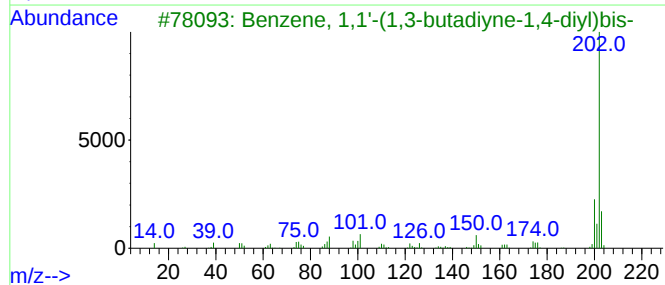
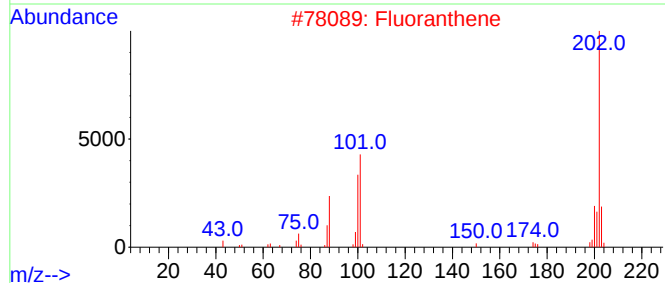
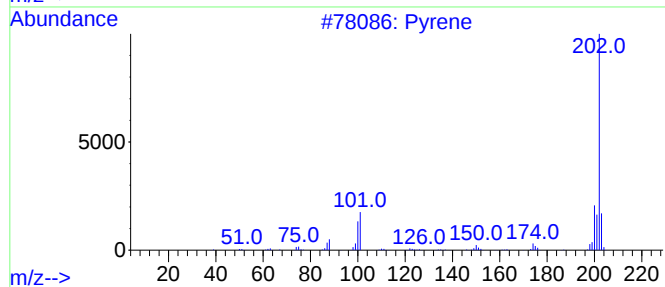
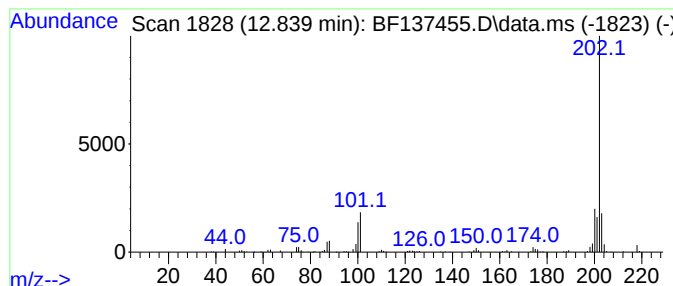
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Peak Number 5 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.839	2.81 ng	166074	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene	202	C16H10	000129-00-0	97
2			Fluoranthene	202	C16H10	000206-44-0	91
3			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	53
4			4,5-Dihydronaphtho(2,1-d)thiazol...	202	C11H10N2S	034176-49-3	42
5			2-pyrazinol, 3-bromo-5,6-dimethyl-	202	C6H7BrN2O	1010396-05-3	38



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ALS Vial : 6 Sample Multiplier: 1

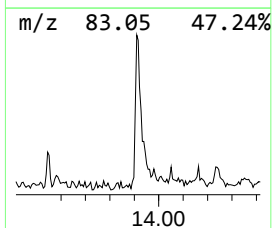
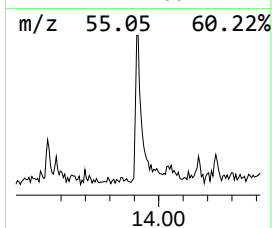
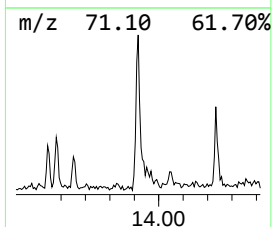
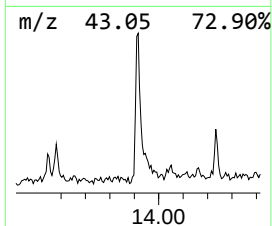
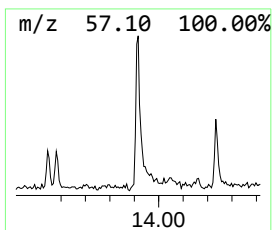
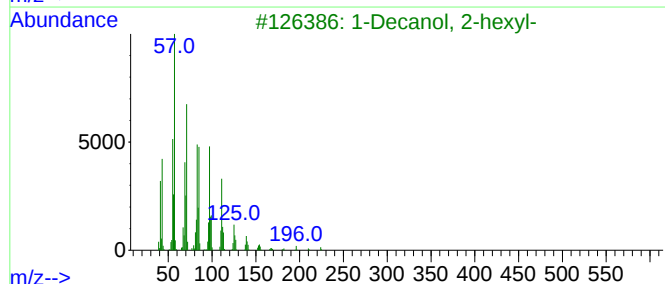
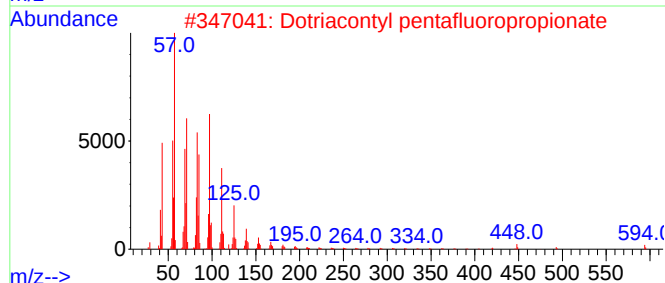
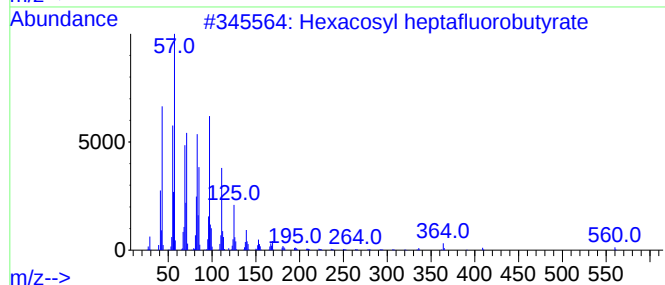
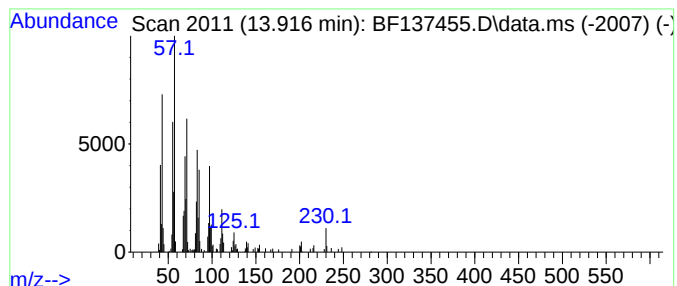
Instrument :
BNA_F
ClientSampleId :
294

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexacosyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.916	3.11 ng	183790	Chrysene-d12		14.051	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexacosyl heptafluorobutyrate		578	C30H53F7O2	1000351-83-3	91
2	Dotriacontyl pentafluoropropionate		612	C35H65F5O2	1010351-81-4	91
3	1-Decanol, 2-hexyl-		242	C16H34O	002425-77-6	91
4	Ethanol, 2-(tetradecyloxy)-		258	C16H34O2	002136-70-1	90
5	Hexacosyl propyl ether		424	C29H60O	1000406-28-4	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030124\
Data File : BF137455.D
Acq On : 01 Mar 2024 13:18
Operator : CG\JU
Sample : P1653-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
294

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.152	27.7	ng	1429020	1	6.869	1030830	20.0
(S)-(+)-1,2-Pro...	3.499	3.4	ng	176520	1	6.869	1030830	20.0
unknown10.004	10.004	13.4	ng	949322	3	9.898	1418390	20.0
n-Hexadecanoic ...	11.939	3.3	ng	202085	4	11.392	1225400	20.0
Benzene, 1,1'-(...	12.839	2.8	ng	166074	5	14.051	1180730	20.0
Hexacosyl hepta...	13.916	3.1	ng	183790	5	14.051	1180730	20.0