

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042624\
Data File : BF137742.D
Acq On : 26 Apr 2024 18:57
Operator : CG\JU
Sample : P2270-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-240

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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-BF042324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137742.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	18	24	31	rVB2	66057	131824	2.63%	0.305%
2	2.446	55	61	66	rBV	385756	505362	10.07%	1.170%
3	3.710	271	276	298	rBV	213138	453597	9.04%	1.050%
4	5.681	606	611	614	rBV	4653075	4256947	84.86%	9.853%
5	6.669	773	779	782	rBV	4502697	4379862	87.31%	10.138%
6	6.869	810	813	820	rBV	101366	91507	1.82%	0.212%
7	7.057	842	845	849	rVB	1879094	1606801	32.03%	3.719%
8	7.616	935	940	944	rBV	2841926	2763779	55.09%	6.397%
9	7.857	977	981	985	rBV	146241	112937	2.25%	0.261%
10	8.345	1059	1064	1067	rBV	2538538	2154355	42.94%	4.986%
11	8.645	1111	1115	1124	rBV	165630	165772	3.30%	0.384%
12	9.416	1241	1246	1249	rBV	5943998	5016608	100.00%	11.611%
13	10.104	1359	1363	1366	rBV	3027595	2426629	48.37%	5.617%
14	10.192	1372	1378	1381	rBV	3164237	3921563	78.17%	9.077%
15	10.892	1493	1497	1501	rBV	3389136	3012682	60.05%	6.973%
16	10.963	1506	1509	1512	rVB	119215	92988	1.85%	0.215%
17	11.598	1613	1617	1620	rBV	2825845	2373277	47.31%	5.493%
18	11.939	1671	1675	1678	rVB	136253	110290	2.20%	0.255%
19	12.104	1695	1703	1713	rBV	747689	774769	15.44%	1.793%
20	12.210	1718	1721	1724	rVV2	133901	114995	2.29%	0.266%
21	12.245	1724	1727	1729	rVB2	81270	64551	1.29%	0.149%
22	12.357	1743	1746	1748	rBV	72107	61053	1.22%	0.141%
23	12.380	1748	1750	1753	rVB	86273	64829	1.29%	0.150%
24	12.486	1766	1768	1773	rVB	74296	59098	1.18%	0.137%
25	12.674	1797	1800	1803	rBV2	81879	74501	1.49%	0.172%
26	12.733	1807	1810	1814	rVB2	168972	148896	2.97%	0.345%
27	12.816	1820	1824	1828	rBV	137664	121835	2.43%	0.282%
28	12.869	1828	1833	1834	rBV3	64352	72900	1.45%	0.169%
29	12.886	1834	1836	1842	rVB3	114412	175927	3.51%	0.407%
30	13.045	1861	1863	1870	rVB2	104945	122653	2.44%	0.284%
31	13.186	1883	1887	1890	rBV	4439300	3980602	79.35%	9.213%
32	14.074	2034	2038	2050	rBV	220386	318324	6.35%	0.737%
33	14.192	2055	2058	2060	rBV	89830	81817	1.63%	0.189%
34	14.245	2063	2067	2071	rBV	1442811	1325131	26.41%	3.067%
35	14.698	2141	2144	2146	rBV3	51391	59177	1.18%	0.137%
36	15.121	2213	2216	2222	rBV	166562	177986	3.55%	0.412%

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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-BF042324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.345	2250	2254	2261	rVB2	47905	84777	1.69%	0.196%
38	15.451	2268	2272	2279	rBV3	70284	140917	2.81%	0.326%
39	15.821	2329	2335	2344	rBV	1156088	1519586	30.29%	3.517%
40	16.398	2428	2433	2440	rBV9	29972	83215	1.66%	0.193%

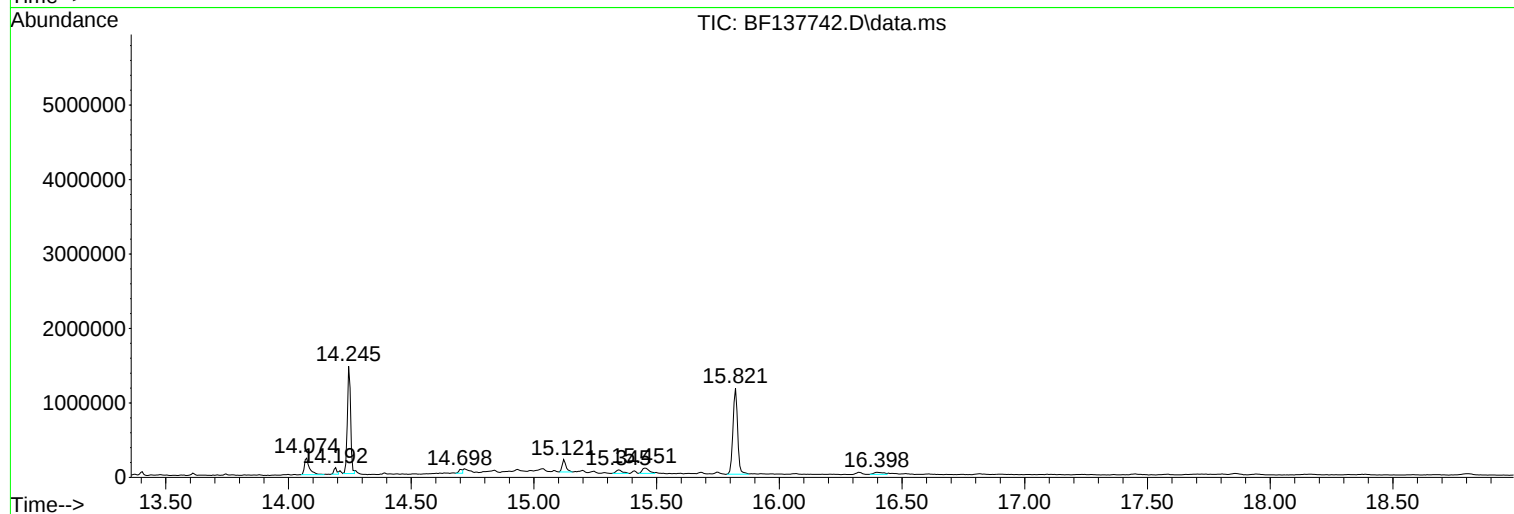
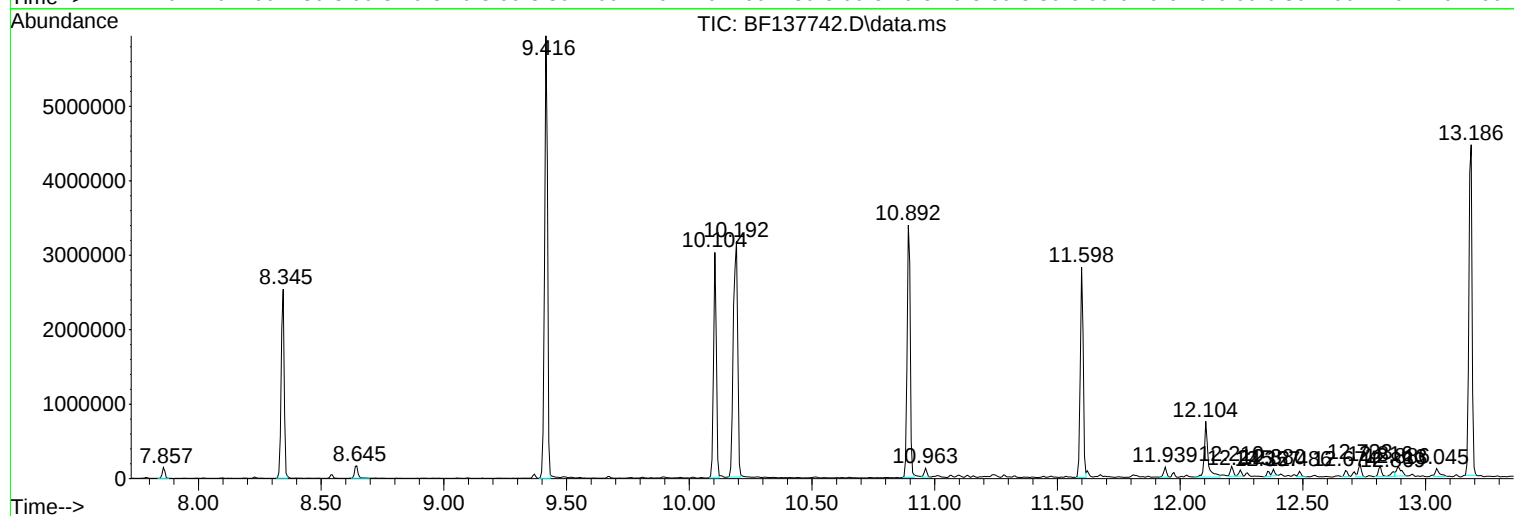
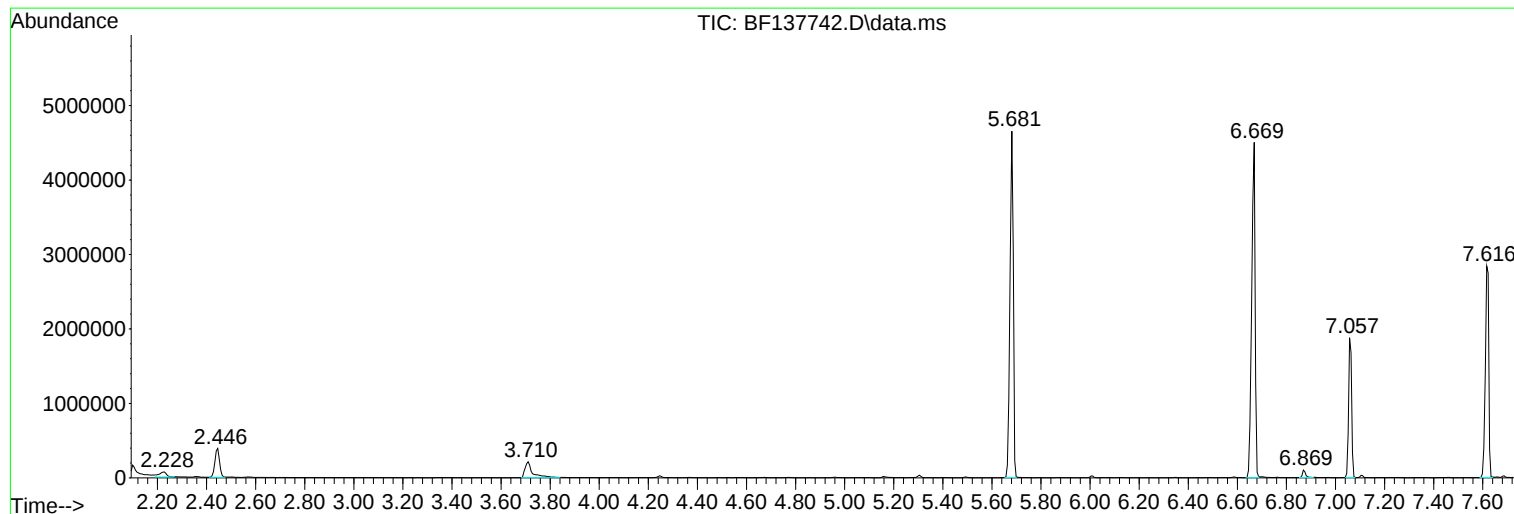
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

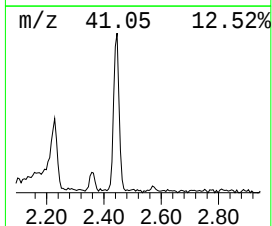
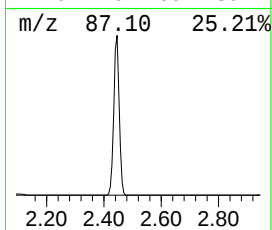
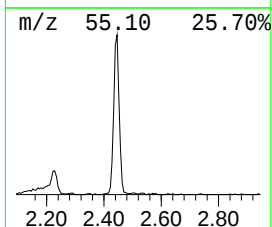
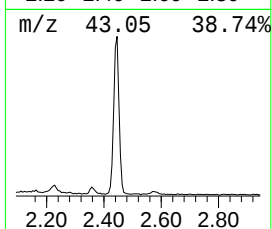
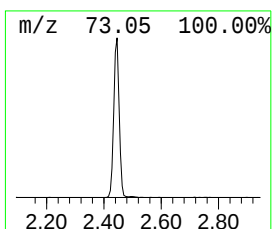
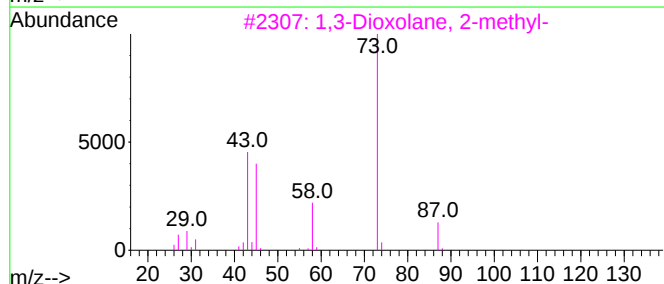
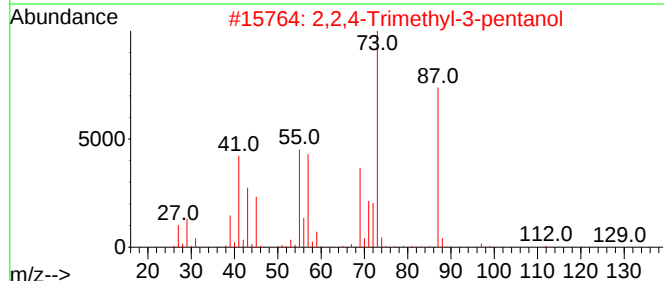
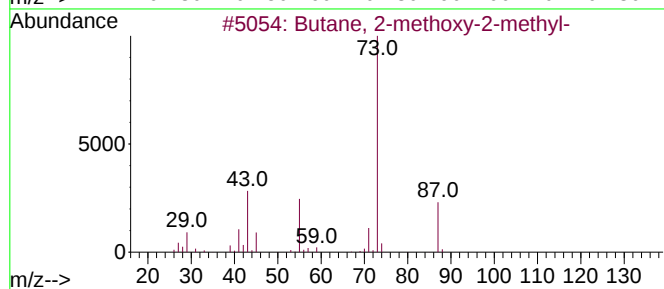
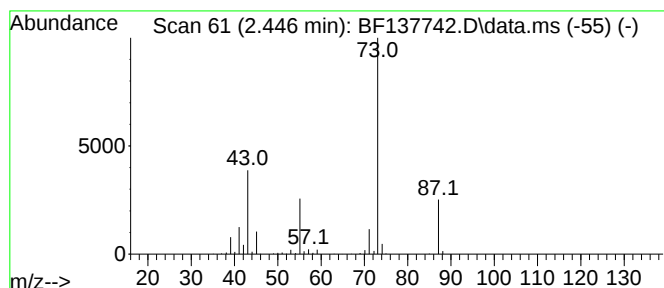
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.446	6.29 ng	505362	1,4-Dichlorobenzene-d4	7.057

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	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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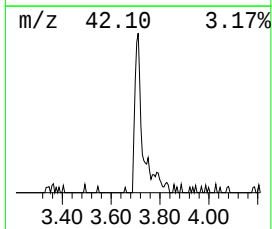
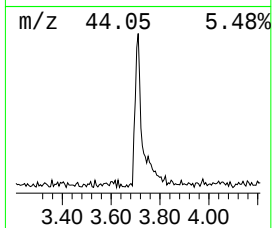
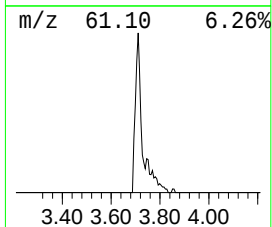
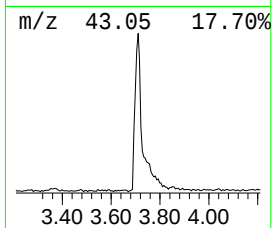
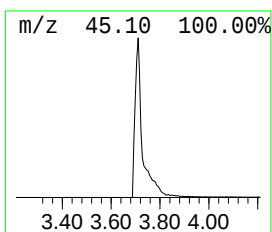
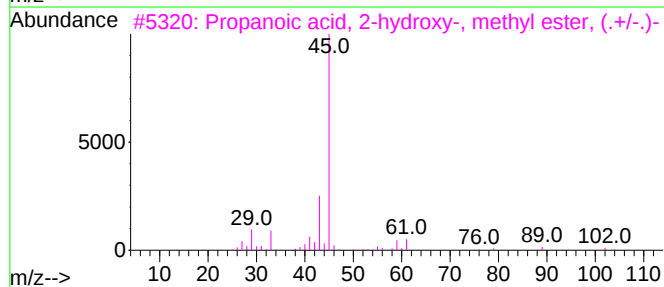
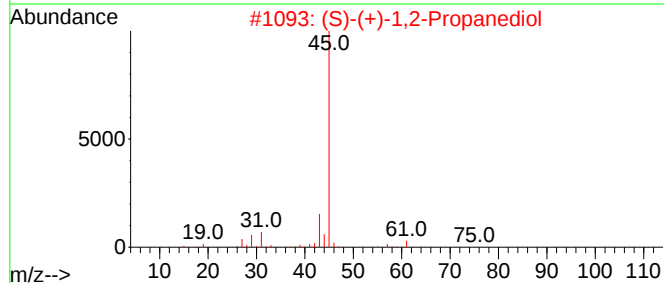
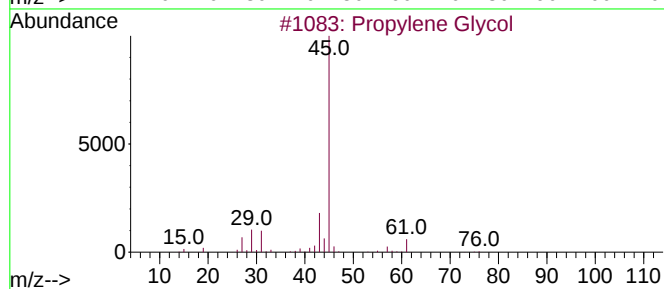
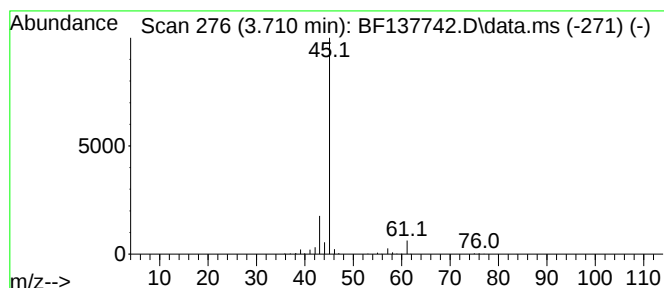
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown3.710 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.710	5.65 ng	453597	1,4-Dichlorobenzene-d4	7.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	47
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	37
5			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	9



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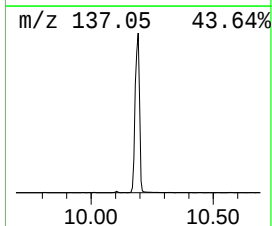
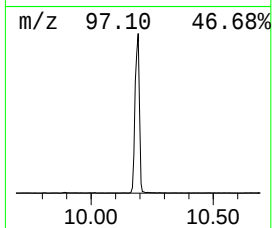
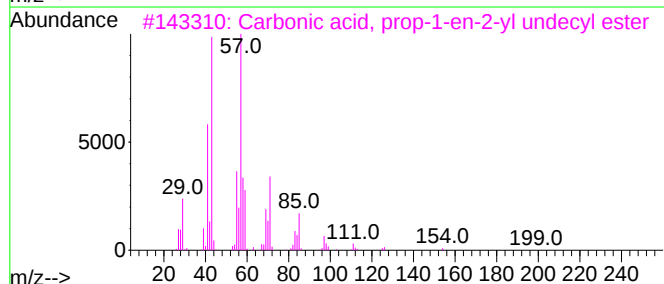
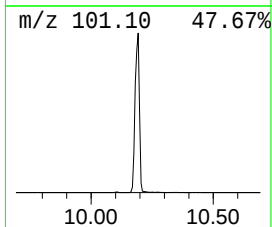
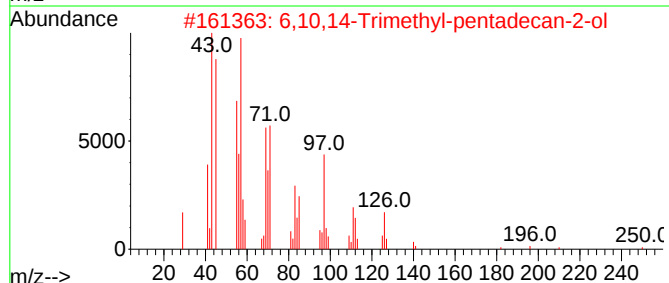
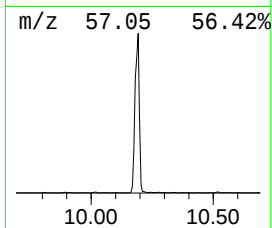
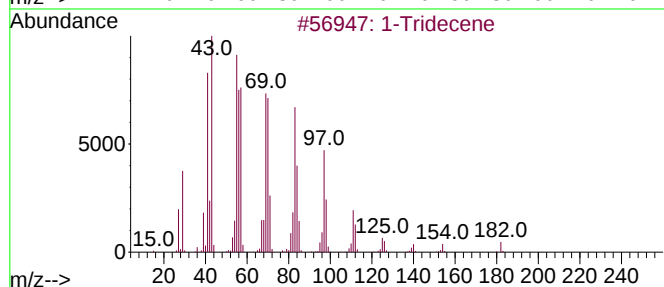
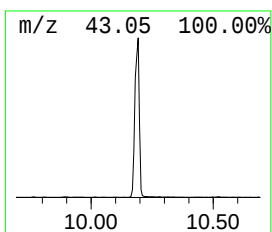
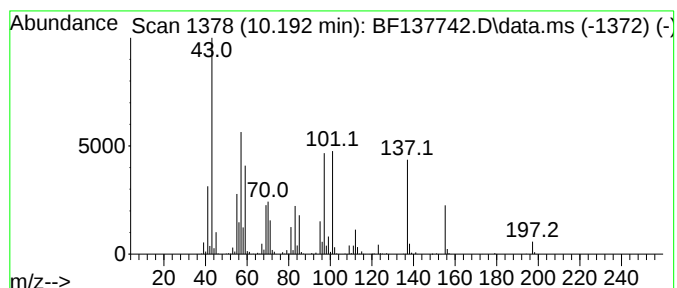
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown10.192 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.192	32.32 ng	3921560	Acenaphthene-d10	10.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tridecene	182	C13H26	002437-56-1	10
2			6,10,14-Trimethyl-pentadecan-2-ol	270	C18H38O	069729-17-5	10
3			Carbonic acid, prop-1-en-2-yl un...	256	C15H28O3	1000382-90-6	10
4			11-Tricosene	322	C23H46	052078-56-5	10
5			Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	10



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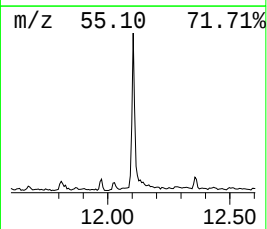
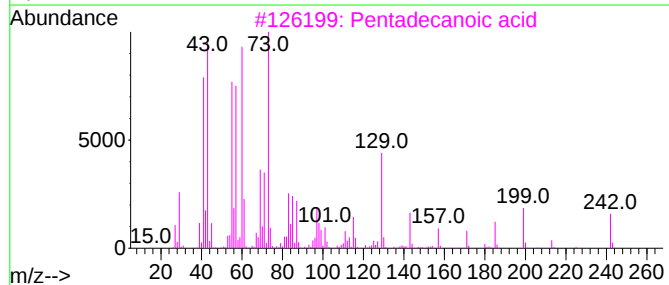
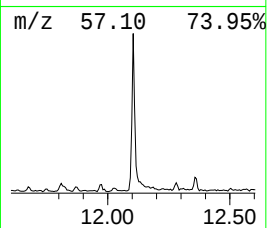
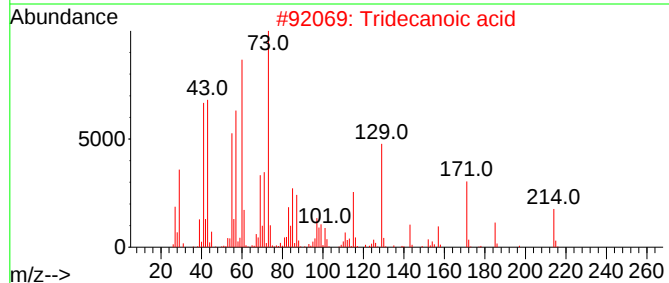
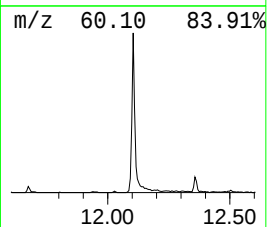
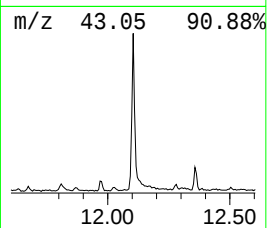
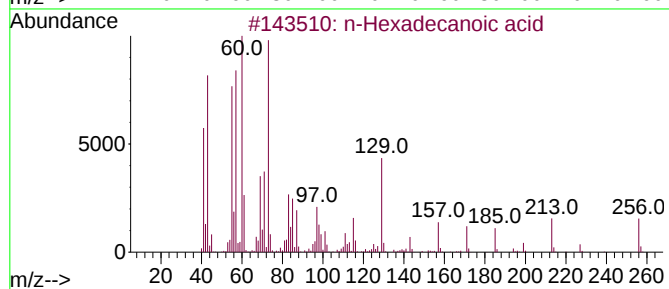
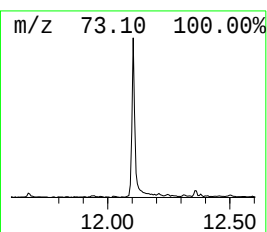
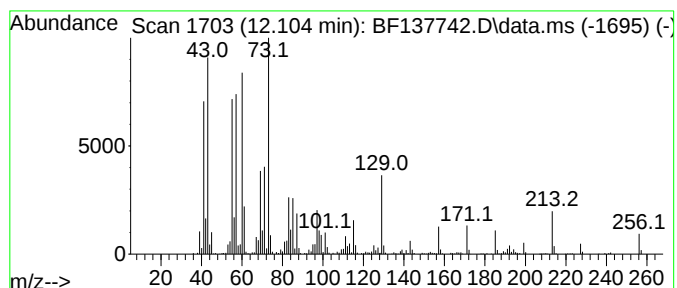
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.104	6.53 ng	774769	Phenanthrene-d10	11.598

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5		Dodecanoic acid	200	C12H24O2	000143-07-7	68



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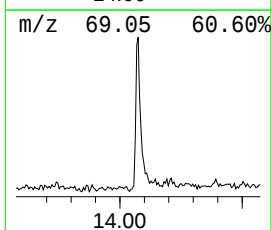
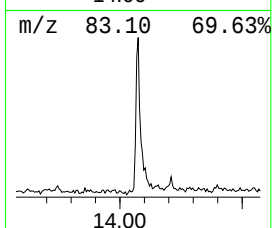
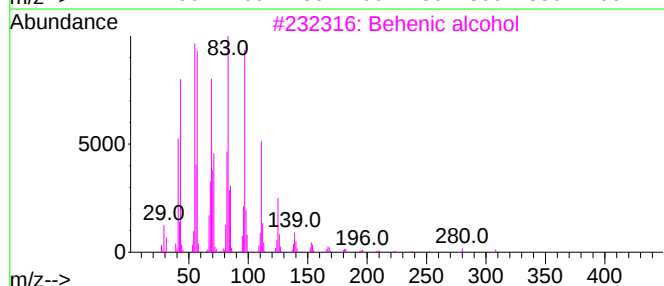
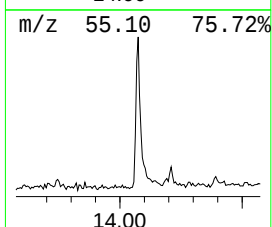
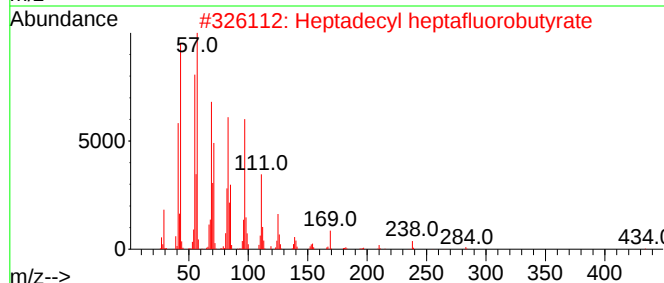
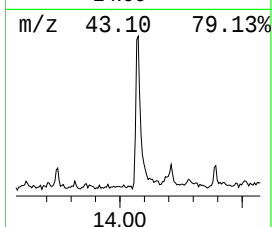
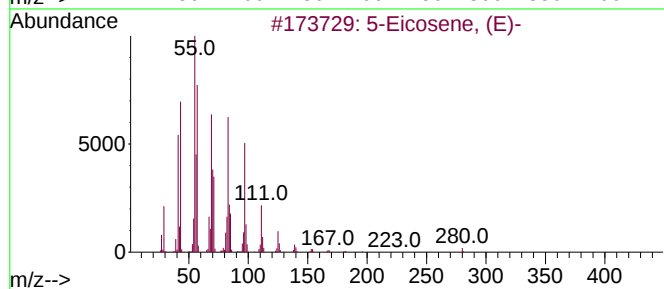
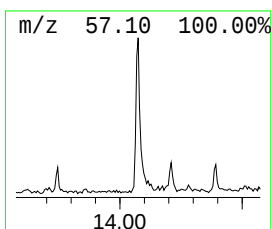
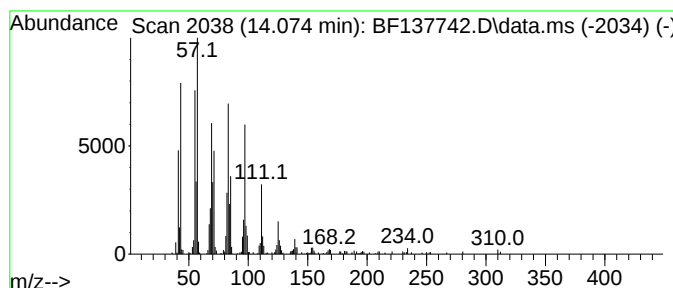
Instrument :
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ClientSampleId :
VNJ-240

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 5-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.074	4.80 ng	318324	Chrysene-d12		14.245	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	96
2	Heptadecyl heptafluorobutyrate		452	C21H35F7O2	959085-66-6	94
3	Behenic alcohol		326	C22H46O	000661-19-8	93
4	Cyclopentadecane		210	C15H30	000295-48-7	93
5	1-Hexacosene		364	C26H52	018835-33-1	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042624\
Data File : BF137742.D
Acq On : 26 Apr 2024 18:57
Operator : CG\JU
Sample : P2270-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-240

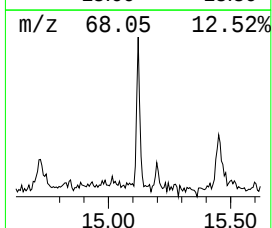
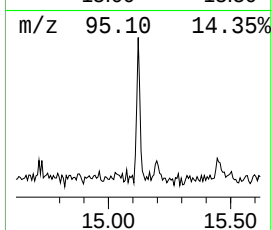
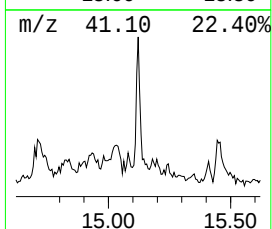
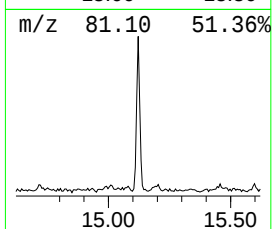
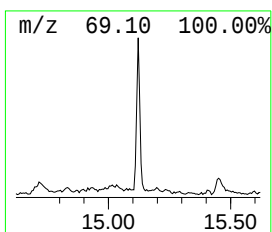
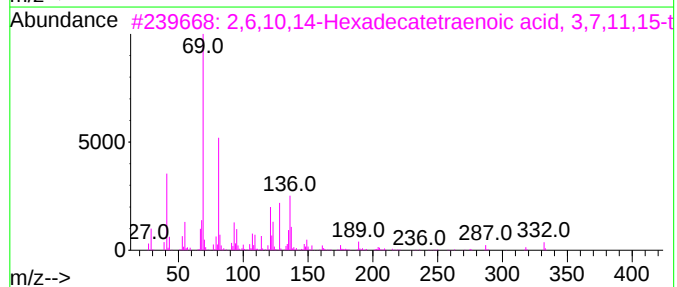
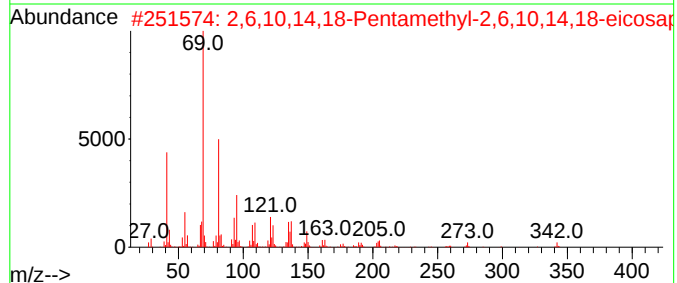
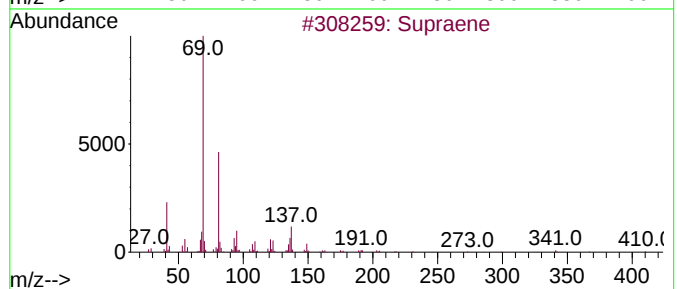
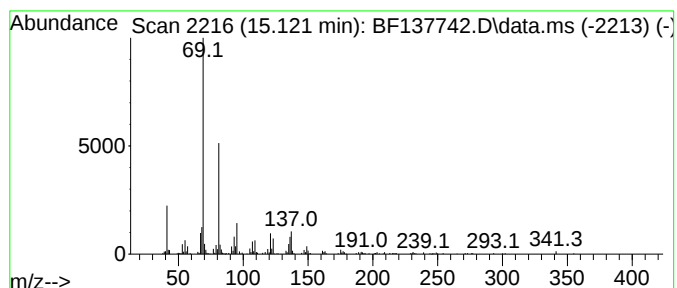
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.121	2.34 ng	177986	Perylene-d12	15.821

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	78
3			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
4			Farnesol isomer a	222	C15H26O	1000108-92-4	64
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042624\
Data File : BF137742.D
Acq On : 26 Apr 2024 18:57
Operator : CG\JU
Sample : P2270-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-240

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.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...	2.446	6.3	ng	505362	1	7.057	1606800	20.0
unknown3.710	3.710	5.7	ng	453597	1	7.057	1606800	20.0
unknown10.192	10.192	32.3	ng	3921560	3	10.104	2426630	20.0
n-Hexadecanoic ...	12.104	6.5	ng	774769	4	11.598	2373280	20.0
5-Eicosene, (E)-	14.074	4.8	ng	318324	5	14.245	1325130	20.0
Supraene	15.121	2.3	ng	177986	6	15.821	1519590	20.0