

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110722\
 Data File : BF131053.D
 Acq On : 07 Nov 2022 20:37
 Operator : CG\JU
 Sample : N5415-06
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 R-19

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-BF110722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131053.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	10	16	23	rBV	616696	761993	38.90%	5.285%
2	2.293	30	35	46	rBV	36807	49224	2.51%	0.341%
3	4.499	407	410	416	rVB	56597	64572	3.30%	0.448%
4	5.122	511	516	530	rVB	392526	456844	23.32%	3.168%
5	5.516	578	583	586	rBV	2055861	1896065	96.78%	13.149%
6	6.522	749	754	757	rBV	1866429	1945849	99.33%	13.495%
7	6.898	814	818	821	rBV	692271	516008	26.34%	3.579%
8	7.463	909	914	917	rBV	1443035	1235092	63.05%	8.566%
9	8.181	1033	1036	1040	rBV	741899	646008	32.98%	4.480%
10	9.263	1215	1220	1223	rBV	2227325	1959057	100.00%	13.586%
11	9.334	1229	1232	1237	rBV2	25205	25532	1.30%	0.177%
12	9.651	1283	1286	1289	rBV4	22158	27498	1.40%	0.191%
13	9.939	1332	1335	1339	rVB	578939	527733	26.94%	3.660%
14	10.733	1466	1470	1473	rBV	971527	803921	41.04%	5.575%
15	10.851	1486	1490	1493	rBV2	20349	26685	1.36%	0.185%
16	11.433	1585	1589	1592	rBV	499382	432695	22.09%	3.001%
17	11.457	1592	1593	1596	rVB	104603	59659	3.05%	0.414%
18	11.963	1677	1679	1682	rVB	28077	24586	1.25%	0.171%
19	12.651	1793	1796	1800	rBV	122422	97105	4.96%	0.673%
20	12.880	1829	1835	1839	rBV	113824	134508	6.87%	0.933%
21	13.022	1855	1859	1863	rBV	1446226	1293241	66.01%	8.969%
22	13.098	1868	1872	1876	rBV4	15660	27602	1.41%	0.191%
23	13.210	1888	1891	1894	rVB	22641	27193	1.39%	0.189%
24	13.316	1905	1909	1914	rBV2	20671	33982	1.73%	0.236%
25	13.921	2009	2012	2015	rBV3	27377	27775	1.42%	0.193%
26	13.969	2015	2020	2024	rVV4	31630	64073	3.27%	0.444%
27	14.080	2035	2039	2042	rBV	447142	440307	22.48%	3.054%
28	14.110	2042	2044	2051	rVB	55730	51484	2.63%	0.357%
29	14.180	2052	2056	2059	rBV3	27065	35111	1.79%	0.243%
30	14.239	2063	2066	2071	rBV5	21102	29783	1.52%	0.207%
31	14.545	2115	2118	2124	rBV3	32864	36006	1.84%	0.250%
32	14.857	2169	2171	2175	rVB4	22985	24248	1.24%	0.168%
33	14.939	2182	2185	2189	rVB	43604	42580	2.17%	0.295%
34	15.139	2215	2219	2222	rBV	53642	83038	4.24%	0.576%
35	15.210	2228	2231	2236	rVB2	54240	60187	3.07%	0.417%
36	15.515	2281	2283	2289	rVB	37664	50428	2.57%	0.350%

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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-BF110722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.586	2290	2295	2303	rVB	288218	401687	20.50%	2.786%
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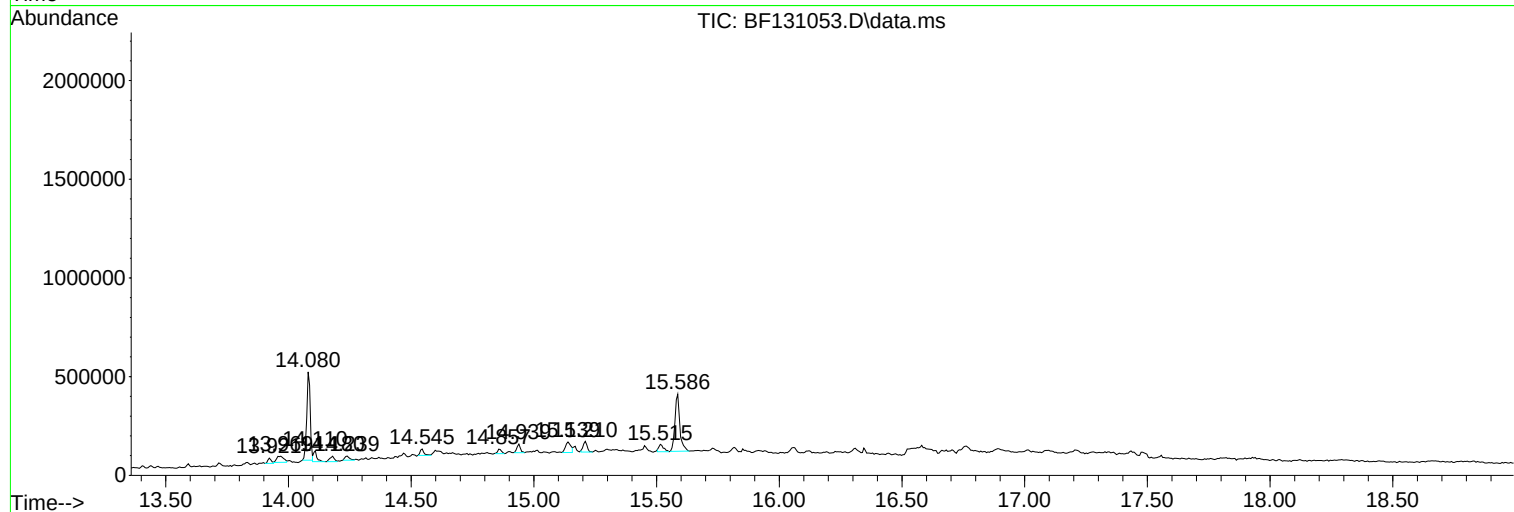
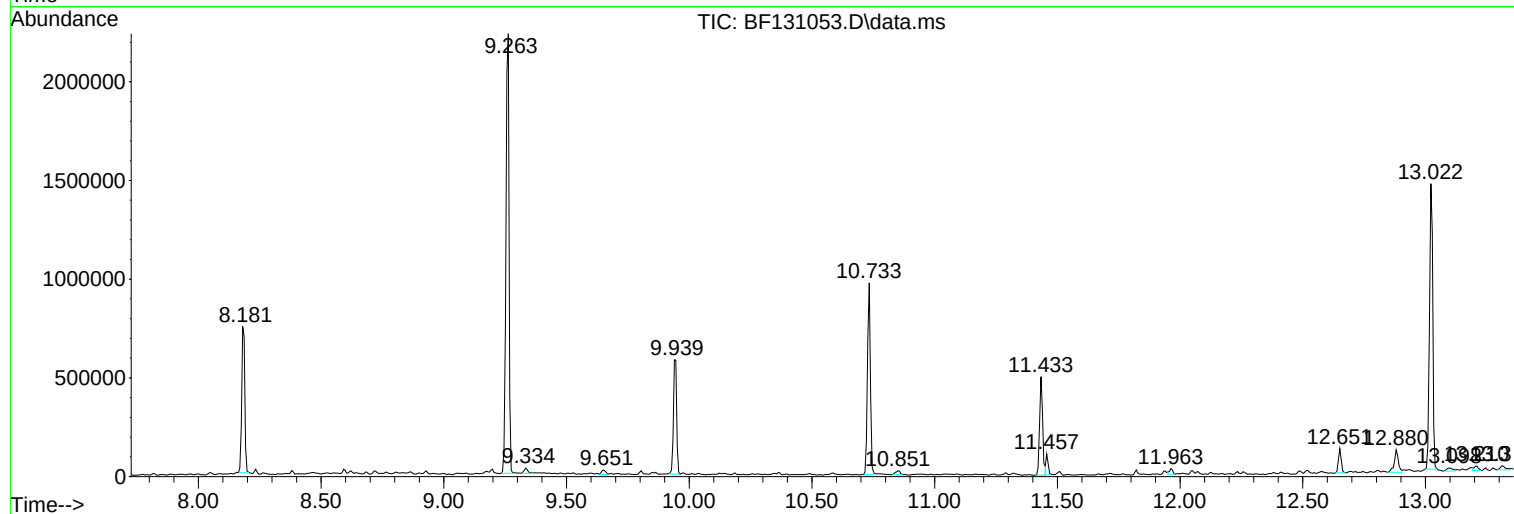
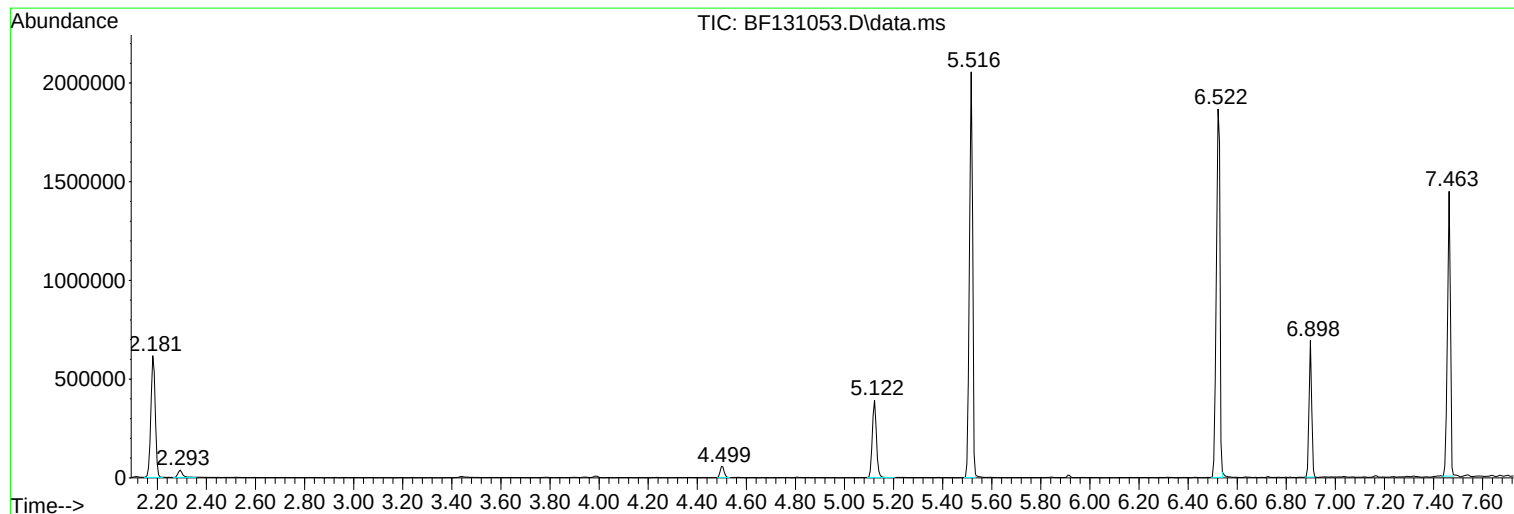
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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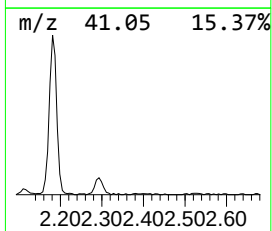
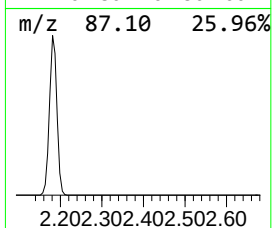
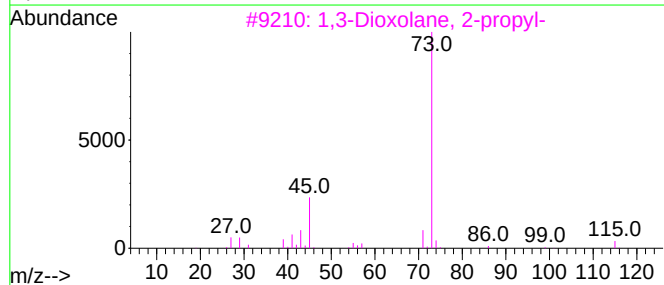
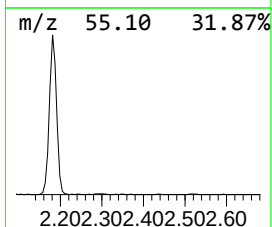
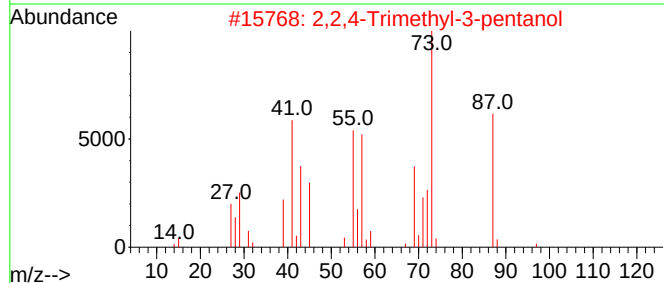
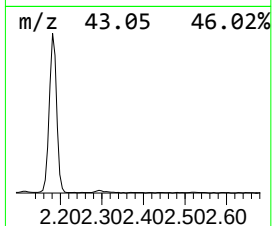
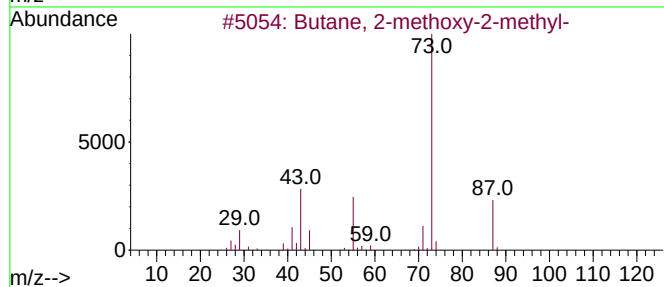
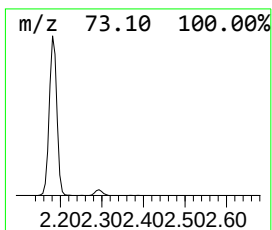
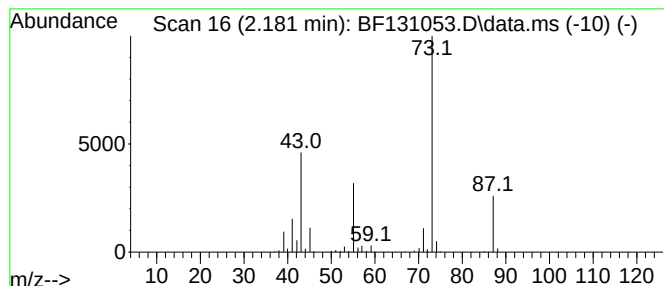
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	29.53 ng	761993	1,4-Dichlorobenzene-d4	6.898

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-propyl-	116	C6H12O2	003390-13-4	23
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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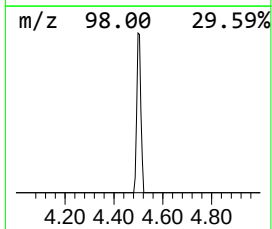
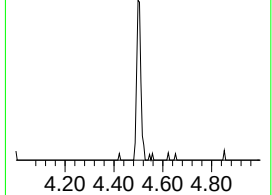
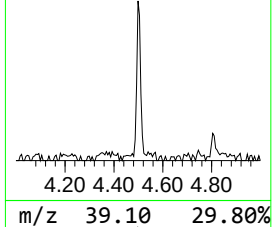
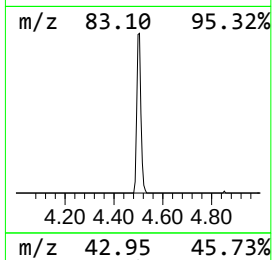
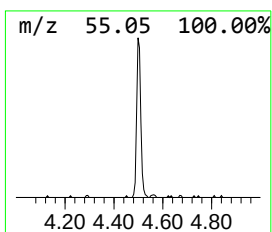
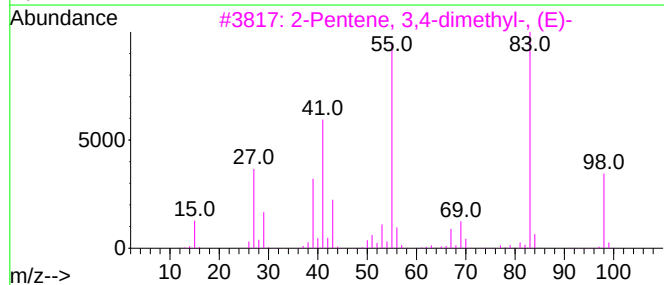
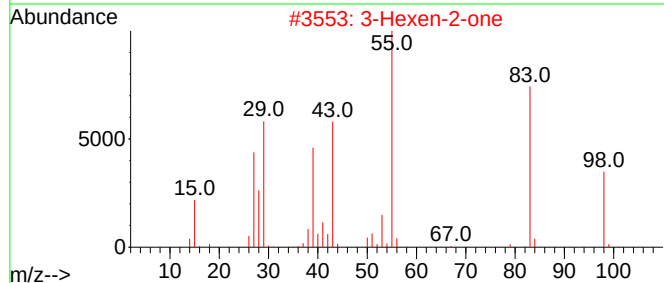
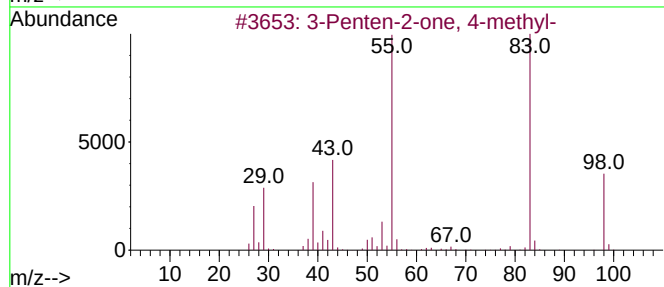
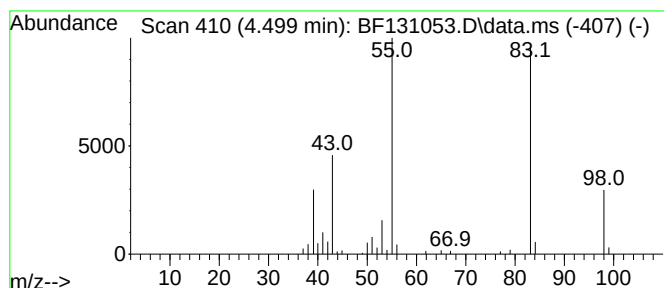
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Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.499	2.50 ng	64572	1,4-Dichlorobenzene-d4	6.898

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86



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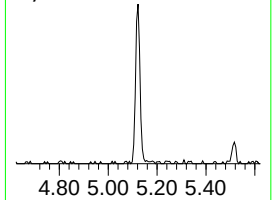
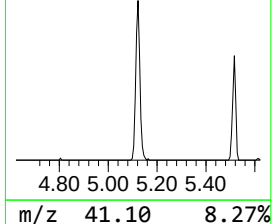
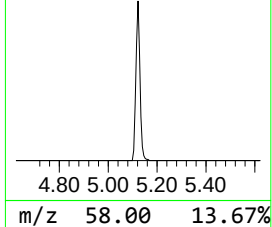
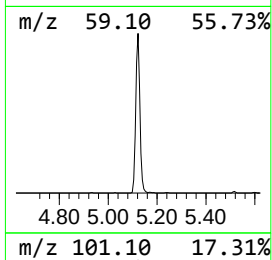
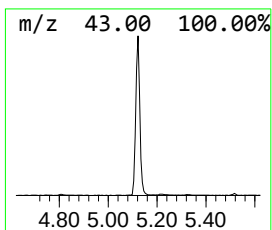
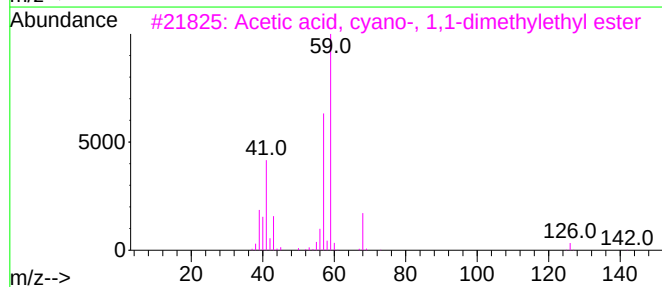
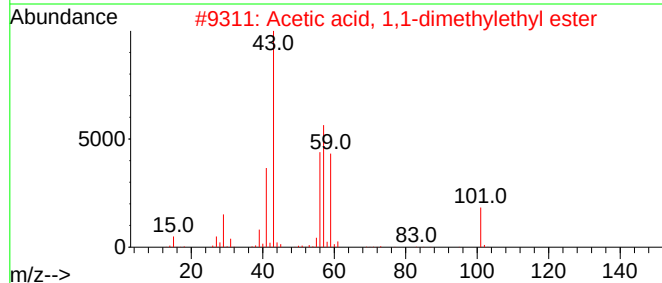
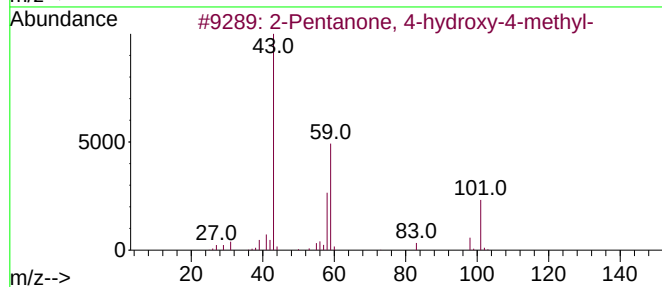
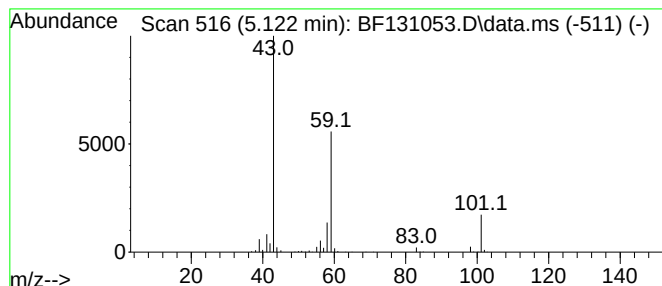
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	17.71 ng	456844	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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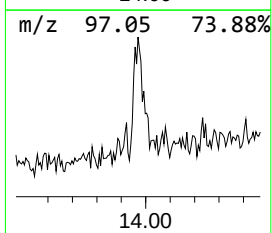
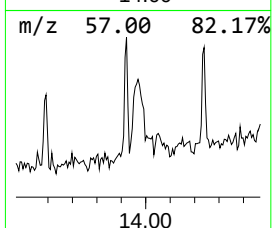
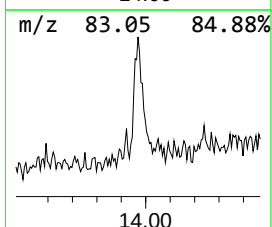
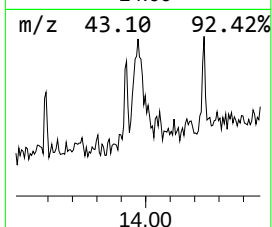
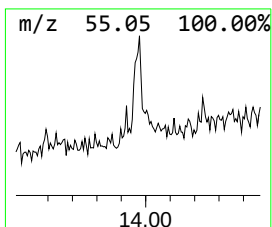
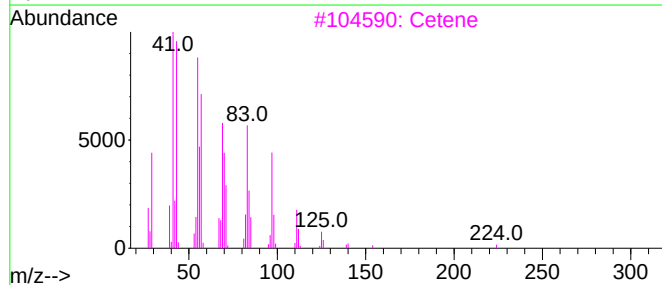
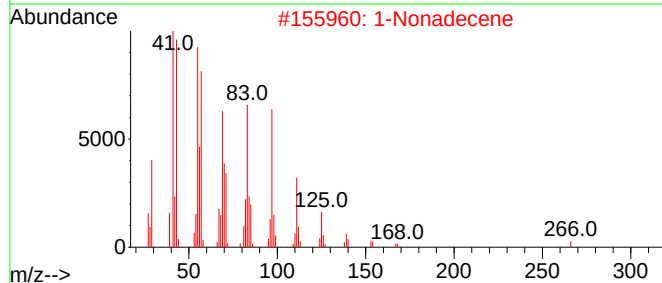
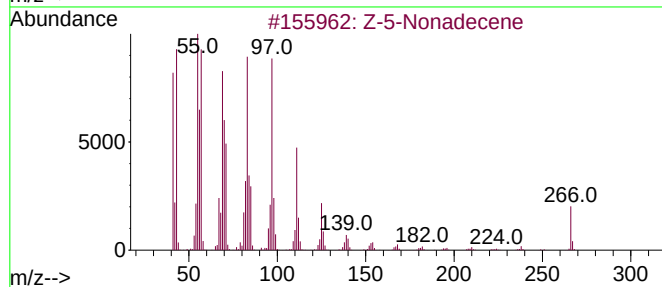
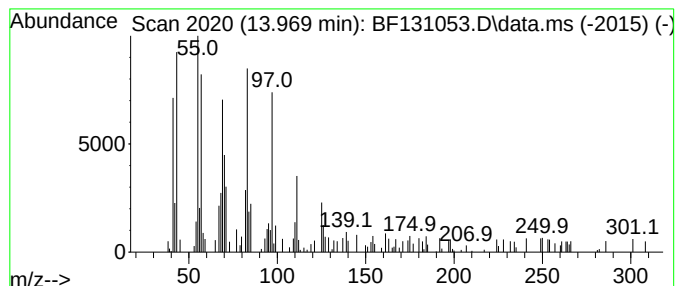
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Z-5-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.969	2.91 ng	64073	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Z-5-Nonadecene	266	C19H38	1000131-11-8	94
2			1-Nonadecene	266	C19H38	018435-45-5	93
3			Cetene	224	C16H32	000629-73-2	90
4			n-Heptadecanol-1	256	C17H36O	001454-85-9	86
5			Carbonic acid, tetradecyl 2,2,2-...	388	C17H31ClO3	1000314-56-0	86



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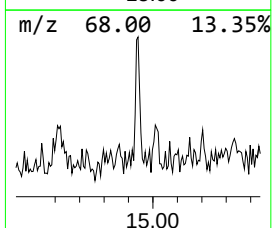
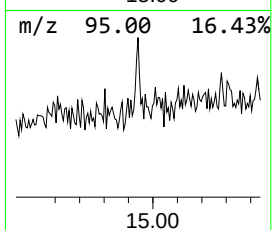
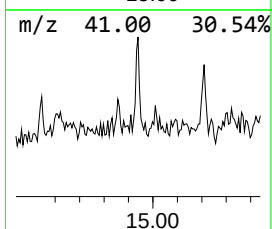
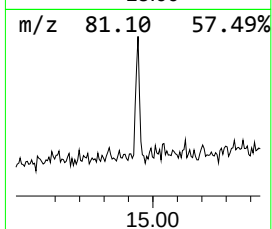
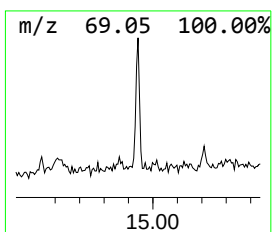
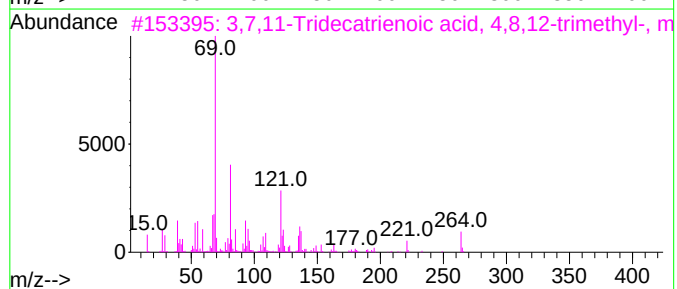
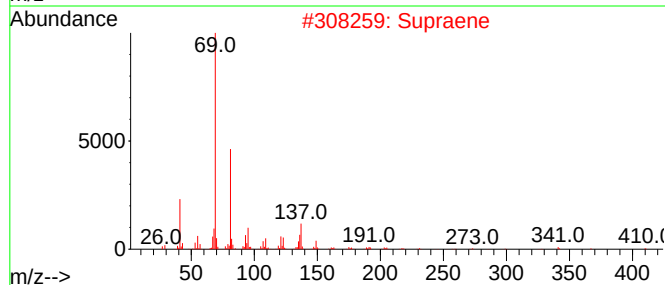
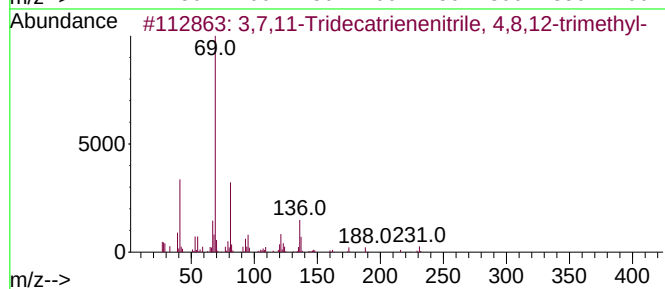
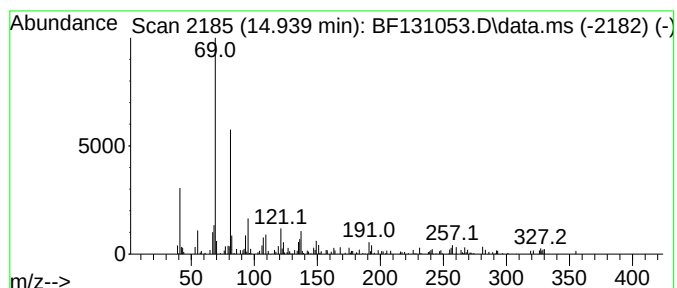
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 3,7,11-Tridecatrienitrile... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.939	2.12 ng	42580	Perylene-d12	15.586	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	72
2	Supraene	410	C30H50	007683-64-9	72
3	3,7,11-Tridecatrienoic acid, 4,8...	264	C17H28O2	036237-70-4	68
4	Umbelliprenin	366	C24H30O3	023838-17-7	64
5	1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110722\
Data File : BF131053.D
Acq On : 07 Nov 2022 20:37
Operator : CG\JU
Sample : N5415-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R-19

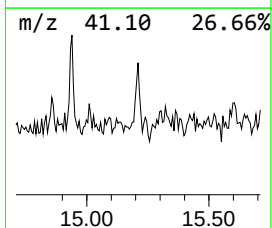
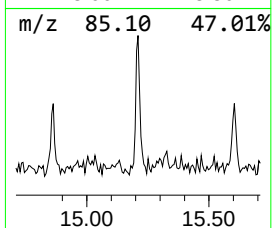
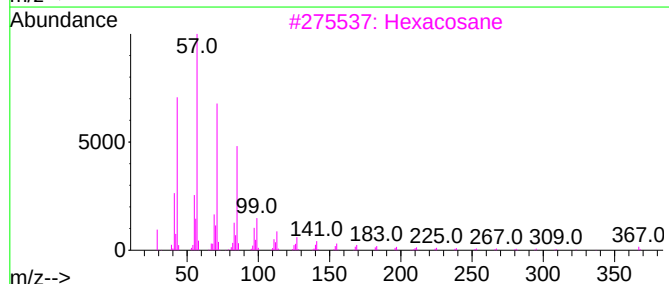
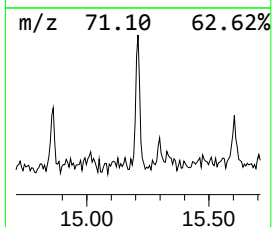
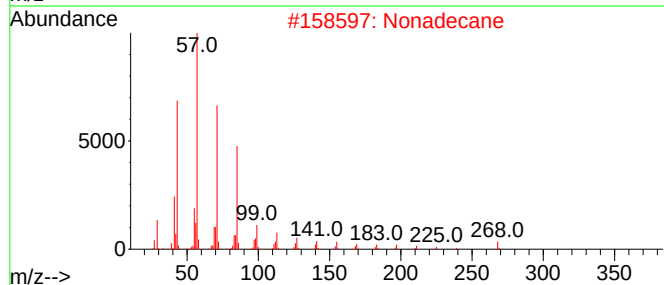
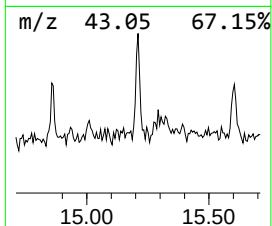
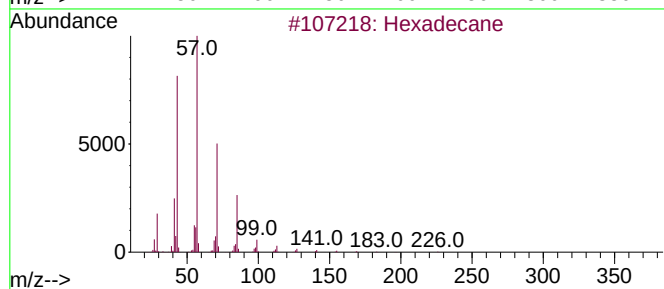
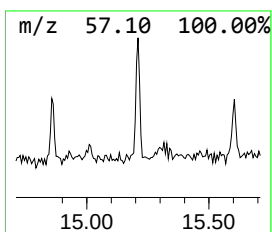
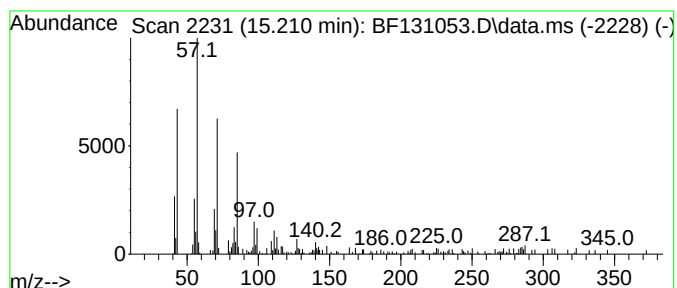
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.210	3.00 ng	60187	Perylene-d12	15.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	95
2			Nonadecane	268	C19H40	000629-92-5	95
3			Hexacosane	366	C26H54	000630-01-3	83
4			Decane, 1-iodo-	268	C10H21I	002050-77-3	76
5			Eicosane	282	C20H42	000112-95-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110722\
Data File : BF131053.D
Acq On : 07 Nov 2022 20:37
Operator : CG\JU
Sample : N5415-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R-19

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110722.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...	2.181	29.5	ng	761993	1	6.898	516008	20.0
3-Penten-2-one,...	4.499	2.5	ng	64572	1	6.898	516008	20.0
2-Pentanone, 4-...	5.122	17.7	ng	456844	1	6.898	516008	20.0
Z-5-Nonadecene	13.969	2.9	ng	64073	5	14.080	440307	20.0
3,7,11-Tridecat...	14.939	2.1	ng	42580	6	15.586	401687	20.0
Hexadecane	15.210	3.0	ng	60187	6	15.586	401687	20.0