

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
 Data File : BF136801.D
 Acq On : 28 Dec 2023 19:18
 Operator : CG\JU
 Sample : 06027-07
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 STONES

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136801.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	8	13	20	rVB2	19237	29069	1.76%	0.262%
2	5.016	494	498	506	rVB	40509	51404	3.11%	0.463%
3	5.422	563	567	577	rBV	1467409	1306646	79.16%	11.763%
4	6.428	733	738	759	rBV	1373837	1357204	82.22%	12.218%
5	6.781	794	798	801	rBV	525208	395859	23.98%	3.564%
6	7.339	889	893	896	rBV	941096	860680	52.14%	7.748%
7	8.057	1011	1015	1018	rBV	647439	500500	30.32%	4.506%
8	9.133	1194	1198	1201	rBV	1966616	1650725	100.00%	14.860%
9	9.680	1287	1291	1293	rBV2	18496	22951	1.39%	0.207%
10	9.722	1295	1298	1301	rVB	39436	34414	2.08%	0.310%
11	9.816	1310	1314	1317	rVB	567001	511098	30.96%	4.601%
12	10.069	1355	1357	1360	rBV2	43307	40558	2.46%	0.365%
13	10.133	1365	1368	1369	rBV3	29319	31610	1.91%	0.285%
14	10.180	1374	1376	1379	rBV3	29796	24005	1.45%	0.216%
15	10.216	1379	1382	1385	rBV2	92863	99927	6.05%	0.900%
16	10.475	1423	1426	1431	rVB	68031	73920	4.48%	0.665%
17	10.610	1445	1449	1452	rBV	854219	795525	48.19%	7.162%
18	10.739	1466	1471	1474	rBV2	371665	452747	27.43%	4.076%
19	11.210	1548	1551	1554	rVB	261980	279702	16.94%	2.518%
20	11.310	1565	1568	1573	rBV	555141	597319	36.19%	5.377%
21	12.904	1836	1839	1847	rVB	1267663	1196916	72.51%	10.775%
22	13.963	2016	2019	2029	rVB	412891	393496	23.84%	3.542%
23	15.439	2266	2270	2275	rBV	297197	364621	22.09%	3.282%
24	16.586	2462	2465	2470	rVB4	23895	37336	2.26%	0.336%

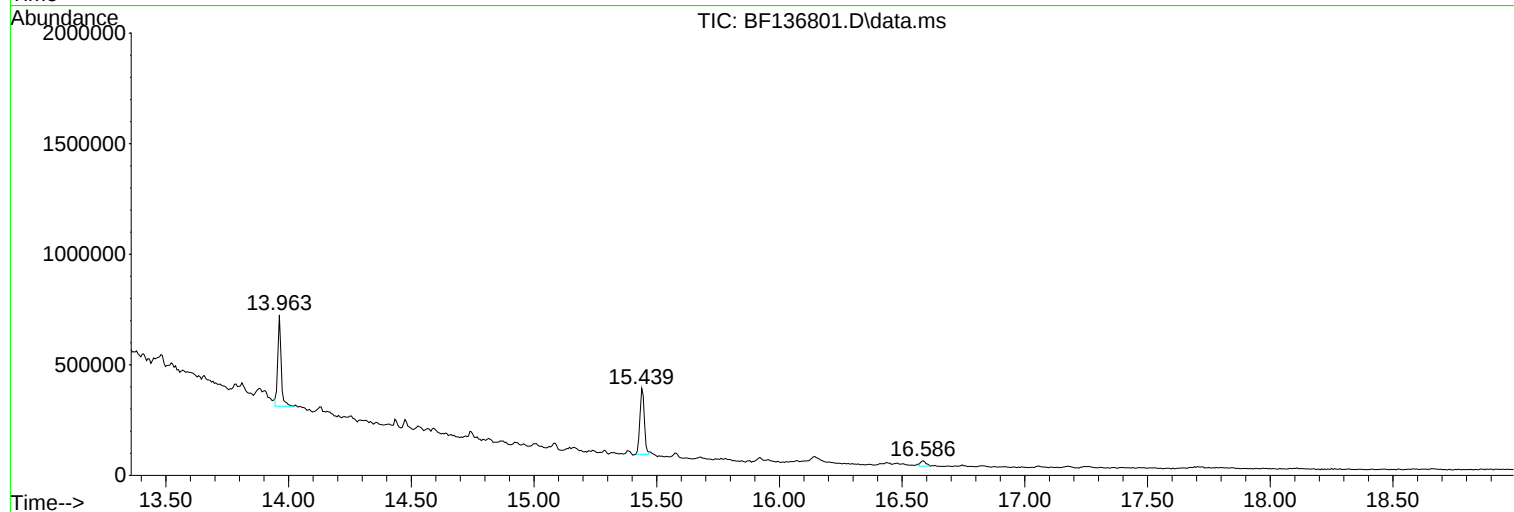
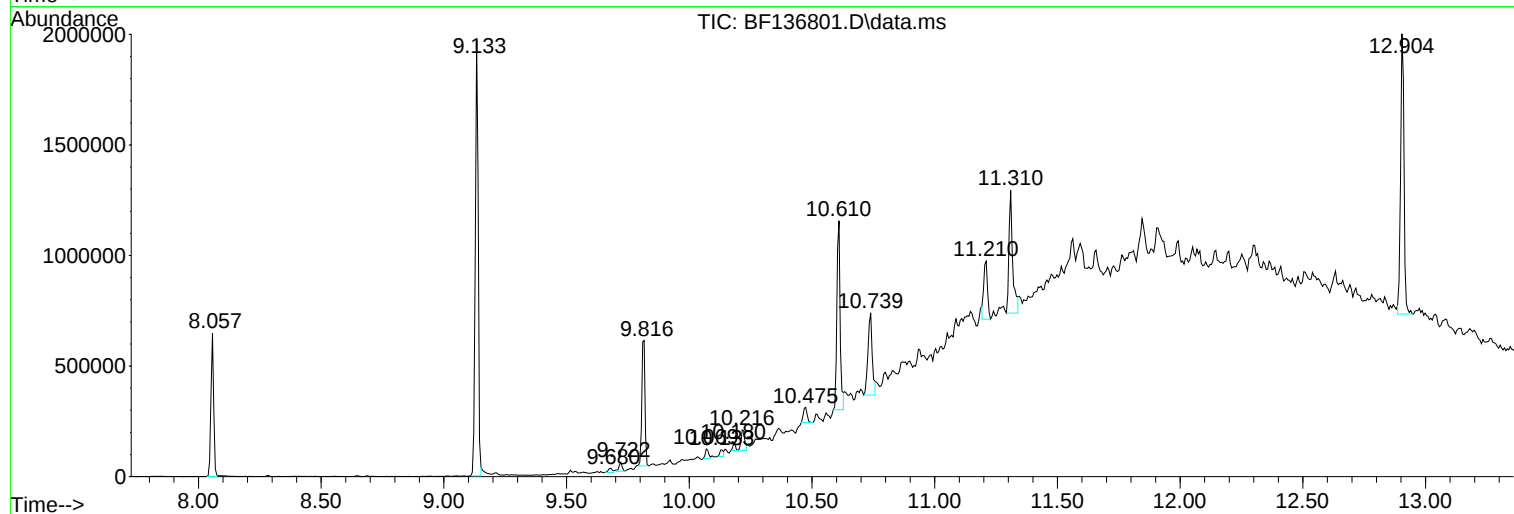
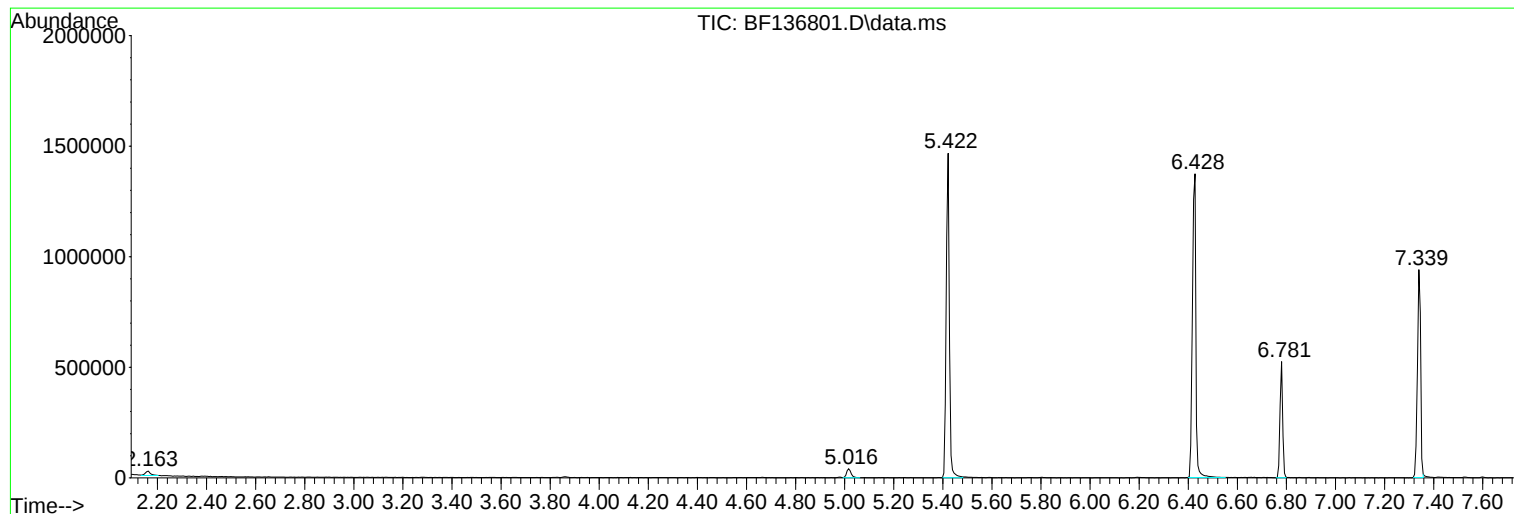
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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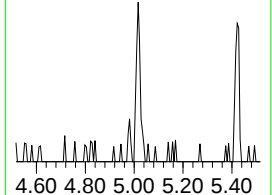
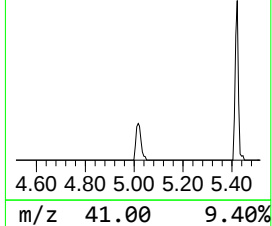
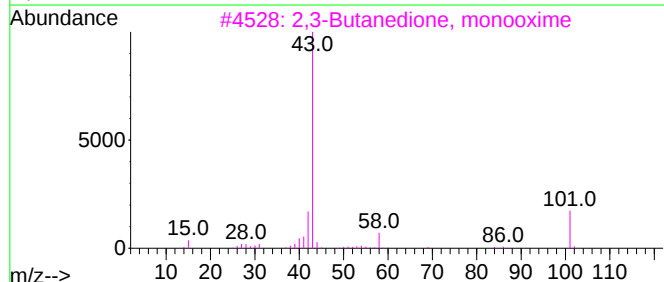
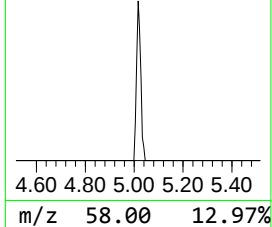
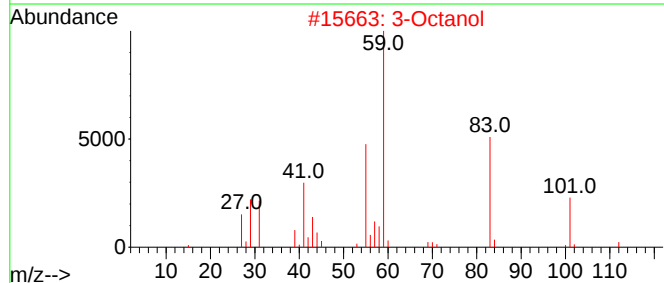
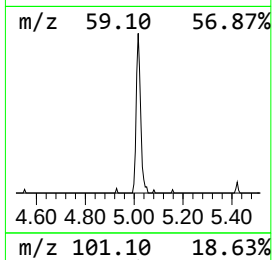
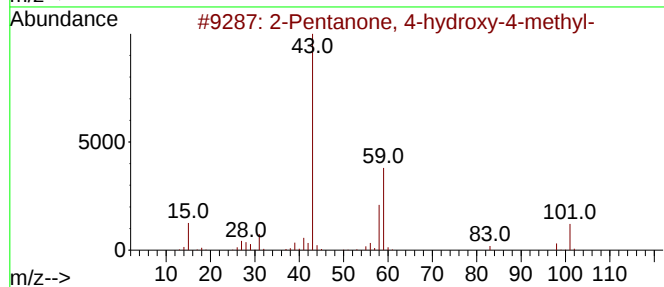
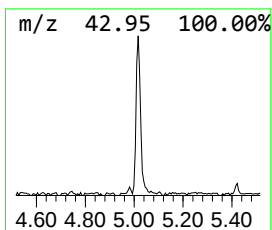
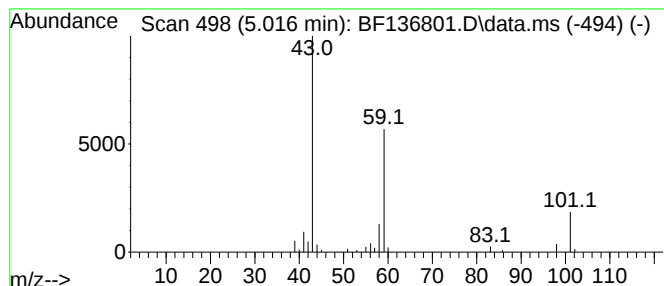
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	2.60 ng	51404	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	3-Octanol	130	C8H18O	000589-98-0	36		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35		
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32		
5	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	23		



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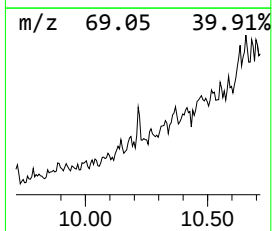
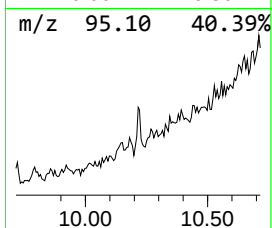
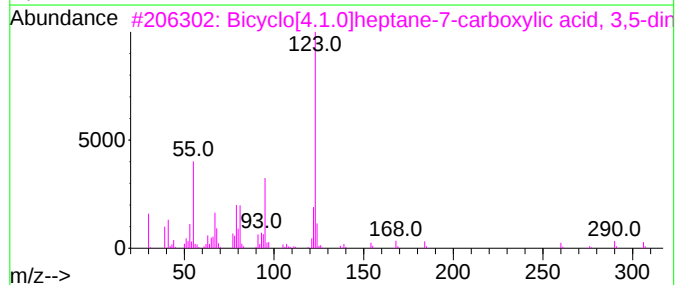
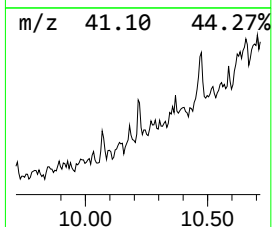
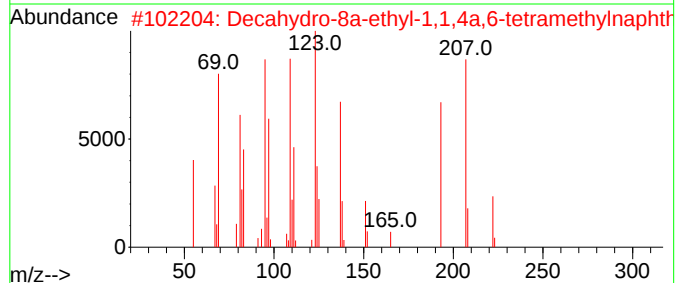
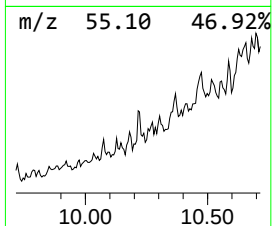
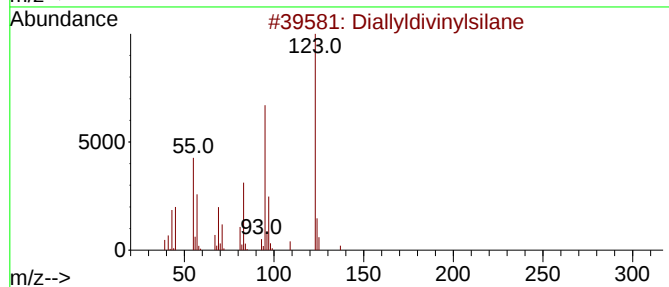
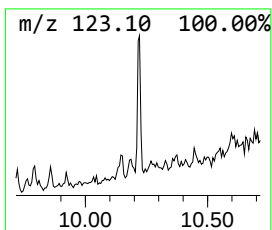
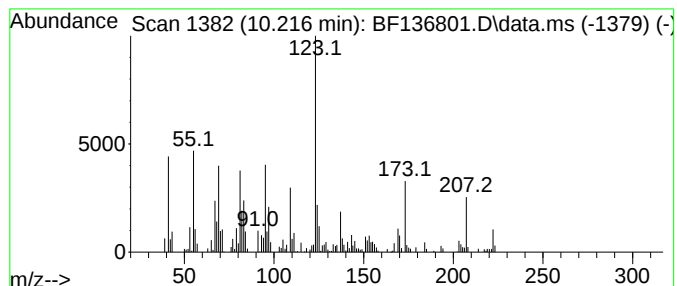
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Peak Number 2 unknown10.216 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.216	3.91 ng	99927	Acenaphthene-d10	9.816

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Diallyldivinylsilane	164	C10H16Si	119901-88-1	47
2		Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	45
3		Bicyclo[4.1.0]heptane-7-carboxyl...	306	C14H14N2O6	1000311-95-8	43
4		3-Fluorobenzoic acid, allyl ester	180	C10H9FO2	1000279-04-2	43
5		4-Fluoro-N-(1H-tetrazol-5-yl)ben...	207	C8H6FN5O	1000306-76-6	38



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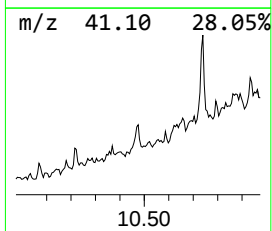
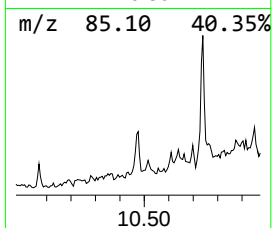
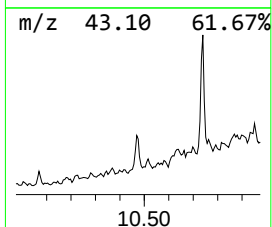
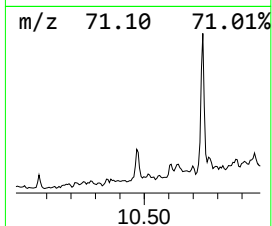
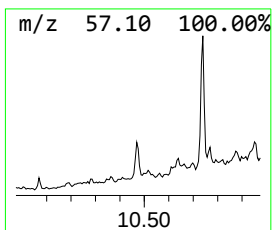
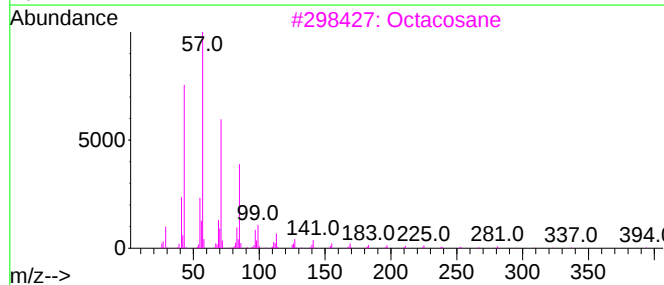
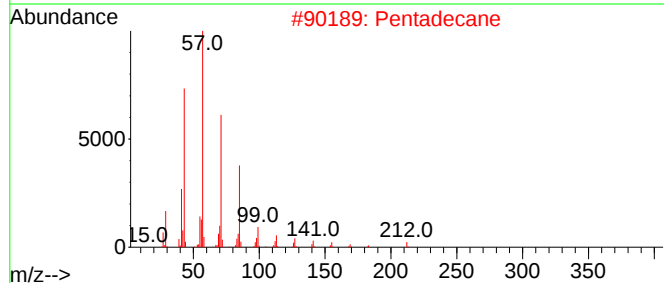
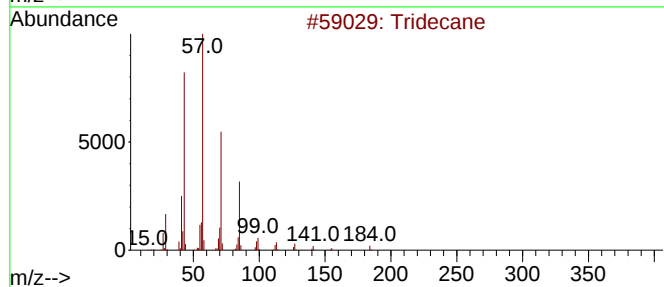
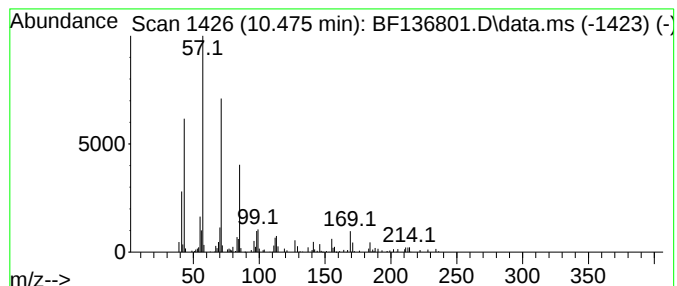
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Peak Number 3 Tridecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	2.89 ng	73920	Acenaphthene-d10	9.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	87
2			Pentadecane	212	C15H32	000629-62-9	72
3			Octacosane	394	C28H58	000630-02-4	72
4			Heptacosane	380	C27H56	000593-49-7	72
5			Decane, 3-methyl-	156	C11H24	013151-34-3	64



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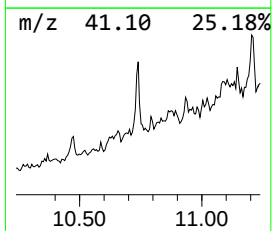
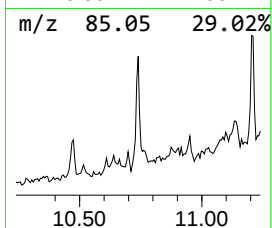
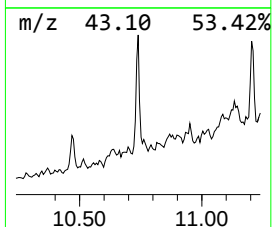
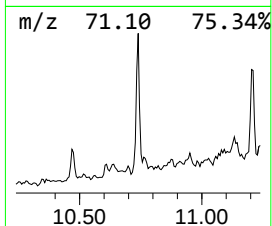
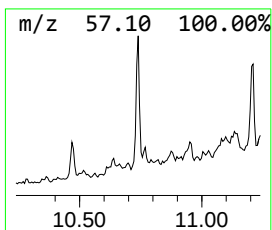
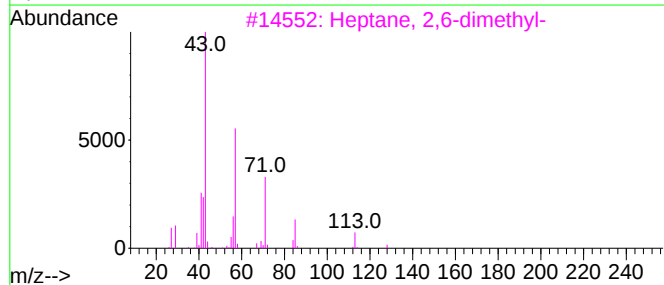
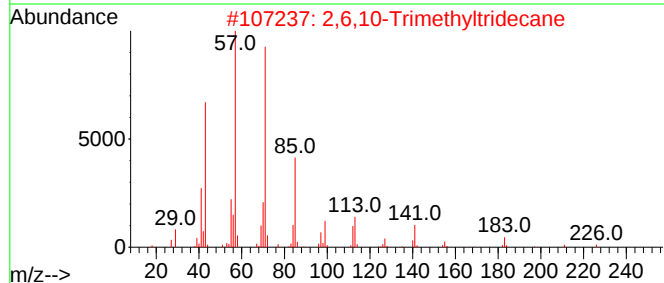
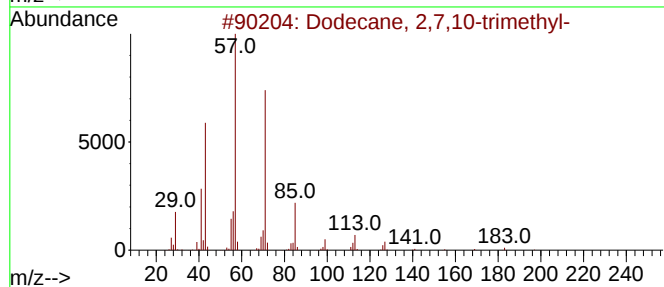
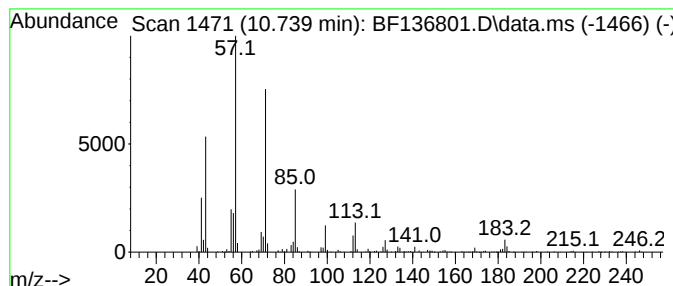
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Peak Number 4 Dodecane, 2,7,10-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.739	15.16 ng	452747	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
2			2,6,10-Trimethyltridecane	226	C16H34	003891-99-4	83
3			Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	74
4			Decane, 3,7-dimethyl-	170	C12H26	017312-54-8	74
5			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72



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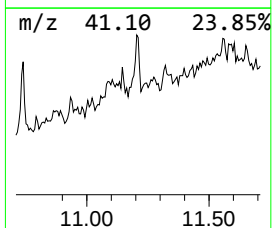
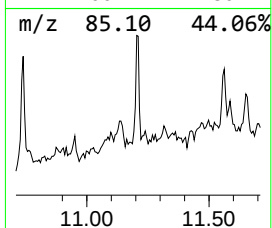
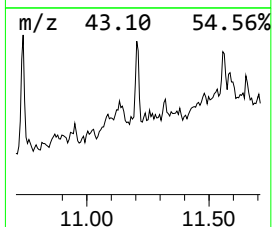
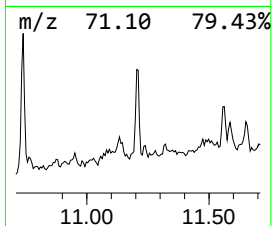
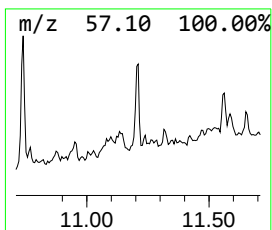
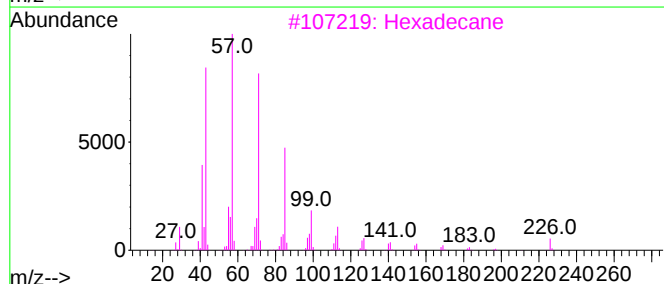
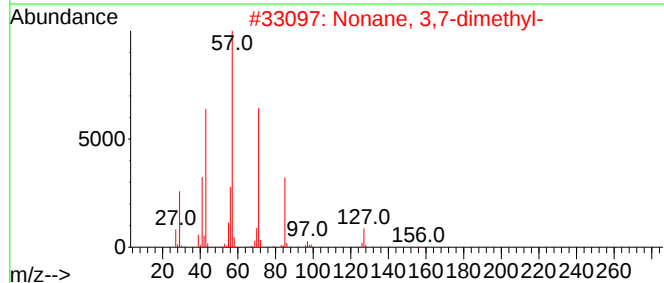
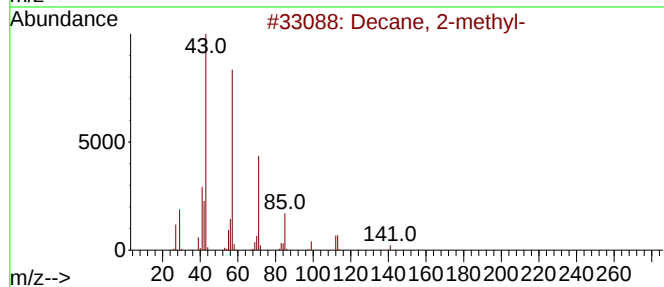
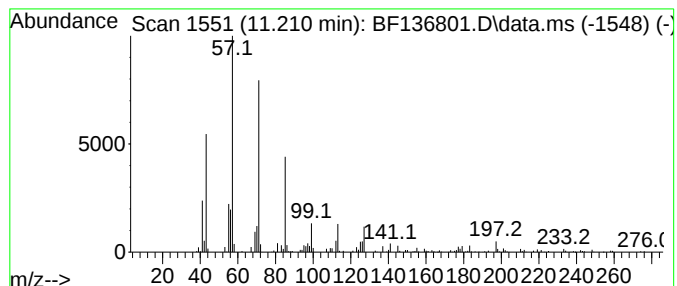
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Peak Number 5 Decane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.210	9.37 ng	279702	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2-methyl-	156	C11H24	006975-98-0	87
2			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	87
3			Hexadecane	226	C16H34	000544-76-3	80
4			Nonadecane	268	C19H40	000629-92-5	72
5			Heptadecane	240	C17H36	000629-78-7	72



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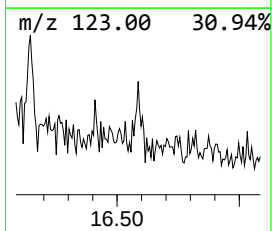
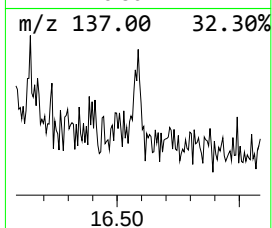
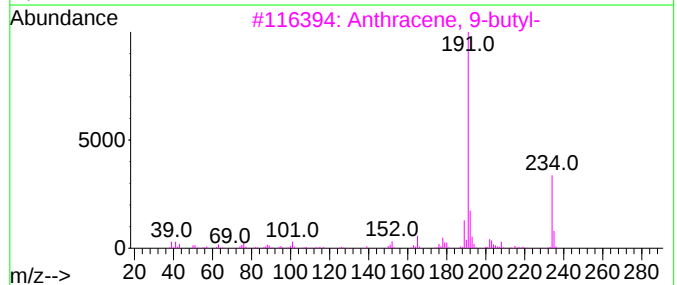
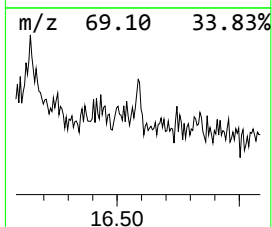
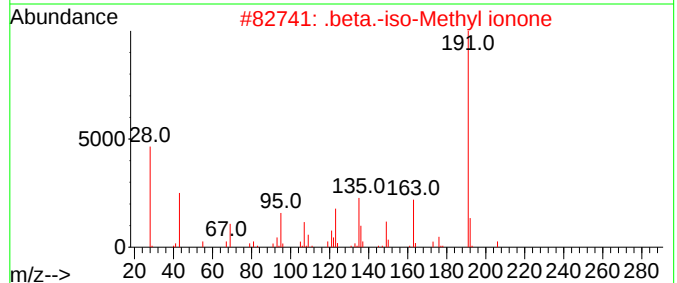
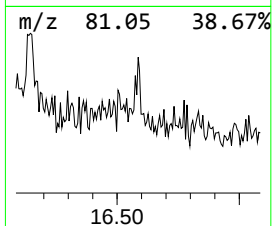
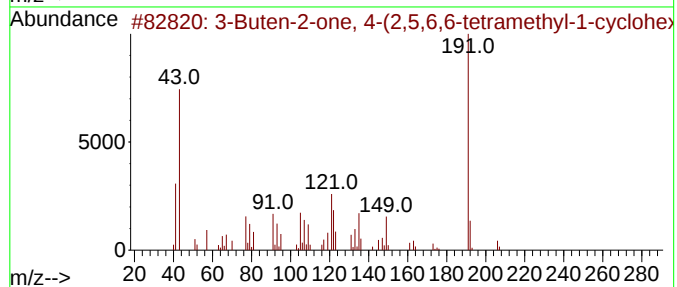
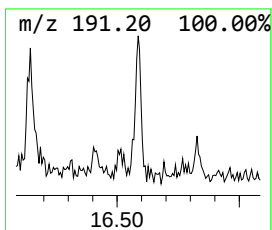
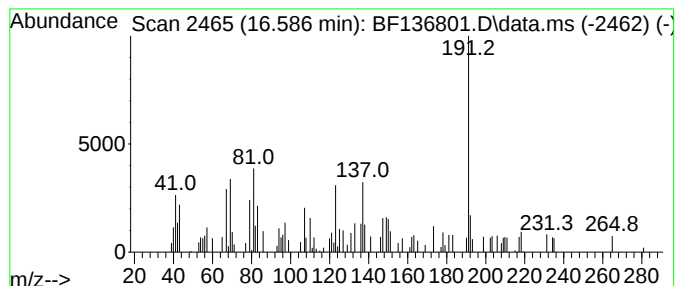
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 3-Buten-2-one, 4-(2,5,6,6-t... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.586	2.05 ng	37336	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Buten-2-one, 4-(2,5,6,6-tetram...	206	C14H22O	000079-70-9	53
2			.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	47
3			Anthracene, 9-butyl-	234	C18H18	001498-69-7	46
4			1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	46
5			3-Methylthio-2-quinoxalinamine	191	C9H9N3S	090349-86-3	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
Data File : BF136801.D
Acq On : 28 Dec 2023 19:18
Operator : CG\JU
Sample : 06027-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STONES

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
2-Pentanone, 4-...	5.016	2.6	ng	51404	1	6.781	395859	20.0
unknown10.216	10.216	3.9	ng	99927	3	9.816	511098	20.0
Tridecane	10.475	2.9	ng	73920	3	9.816	511098	20.0
Dodecane, 2,7,1...	10.739	15.2	ng	452747	4	11.310	597319	20.0
Decane, 2-methyl-	11.210	9.4	ng	279702	4	11.310	597319	20.0
3-Buten-2-one, ...	16.586	2.0	ng	37336	6	15.439	364621	20.0