

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
 Data File : BF113578.D
 Acq On : 4 Apr 2019 8:41
 Operator : JU/SJ
 Sample : K2231-01
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RICH-REC-ROAD-STONE-13

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-BF040319.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.204	356	360	369	rBV	342864	457945	19.24%	2.198%
2	4.863	468	472	488	rBV	555403	678960	28.53%	3.259%
3	5.298	543	546	574	rBV	848758	1004692	42.22%	4.822%
4	5.616	597	600	611	rBV	25502	33810	1.42%	0.162%
5	5.728	616	619	637	rBV	16148	34983	1.47%	0.168%
6	6.334	718	722	740	rBV	1794803	1779956	74.80%	8.543%
7	6.457	740	743	754	rVB	1489134	1274353	53.55%	6.116%
8	6.686	778	782	792	rBV	704103	589169	24.76%	2.828%
9	6.839	805	808	818	rBV	1658486	1563432	65.70%	7.504%
10	7.245	874	877	889	rBV	1065616	1106416	46.49%	5.310%
11	7.333	889	892	906	rVB	79289	90338	3.80%	0.434%
12	7.969	996	1000	1006	rBV	738793	657233	27.62%	3.154%
13	9.045	1179	1183	1195	rBV	2379663	2046405	85.99%	9.822%
14	9.445	1247	1251	1255	rBV	69035	65638	2.76%	0.315%
15	9.722	1294	1298	1308	rVB	776396	688701	28.94%	3.305%
16	10.516	1428	1433	1441	rBV	115349	129272	5.43%	0.620%
17	11.204	1547	1550	1553	rBV	826759	742840	31.22%	3.565%
18	11.227	1553	1554	1558	rVB	98945	68316	2.87%	0.328%
19	11.745	1638	1642	1644	rBV4	22774	31047	1.30%	0.149%
20	11.768	1644	1646	1649	rVV	52764	49186	2.07%	0.236%
21	11.821	1652	1655	1661	rVB2	18422	33506	1.41%	0.161%
22	12.263	1727	1730	1732	rBV3	25144	32335	1.36%	0.155%
23	12.298	1734	1736	1742	rVB2	35790	49532	2.08%	0.238%
24	12.415	1753	1756	1759	rBV	131511	124370	5.23%	0.597%
25	12.645	1791	1795	1797	rBV2	133178	125045	5.25%	0.600%
26	12.668	1797	1799	1802	rVB	52573	48706	2.05%	0.234%
27	12.792	1815	1820	1823	rBV	2454262	2379740	100.00%	11.422%
28	13.027	1857	1860	1864	rBV2	71442	70940	2.98%	0.340%
29	13.368	1916	1918	1921	rVB	98552	78584	3.30%	0.377%
30	13.698	1970	1974	1986	rBV	252021	442041	18.58%	2.122%
31	13.839	1993	1998	2002	rBV2	734514	972228	40.85%	4.666%
32	14.009	2025	2027	2031	rBV	103425	103049	4.33%	0.495%
33	14.315	2077	2079	2082	rBV	142734	130880	5.50%	0.628%
34	14.468	2103	2105	2110	rBV	95210	93460	3.93%	0.449%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.609	2127	2129	2133	rBV	185804	206526	8.68%	0.991%
36	14.680	2138	2141	2145	rVB	227795	249928	10.50%	1.200%
37	14.927	2180	2183	2186	rVB	196982	217499	9.14%	1.044%
38	15.256	2235	2239	2247	rVB2	429985	726632	30.53%	3.487%
39	16.062	2372	2376	2385	rBV2	609572	1400935	58.87%	6.724%
40	16.750	2489	2493	2499	rVB2	155034	256783	10.79%	1.232%

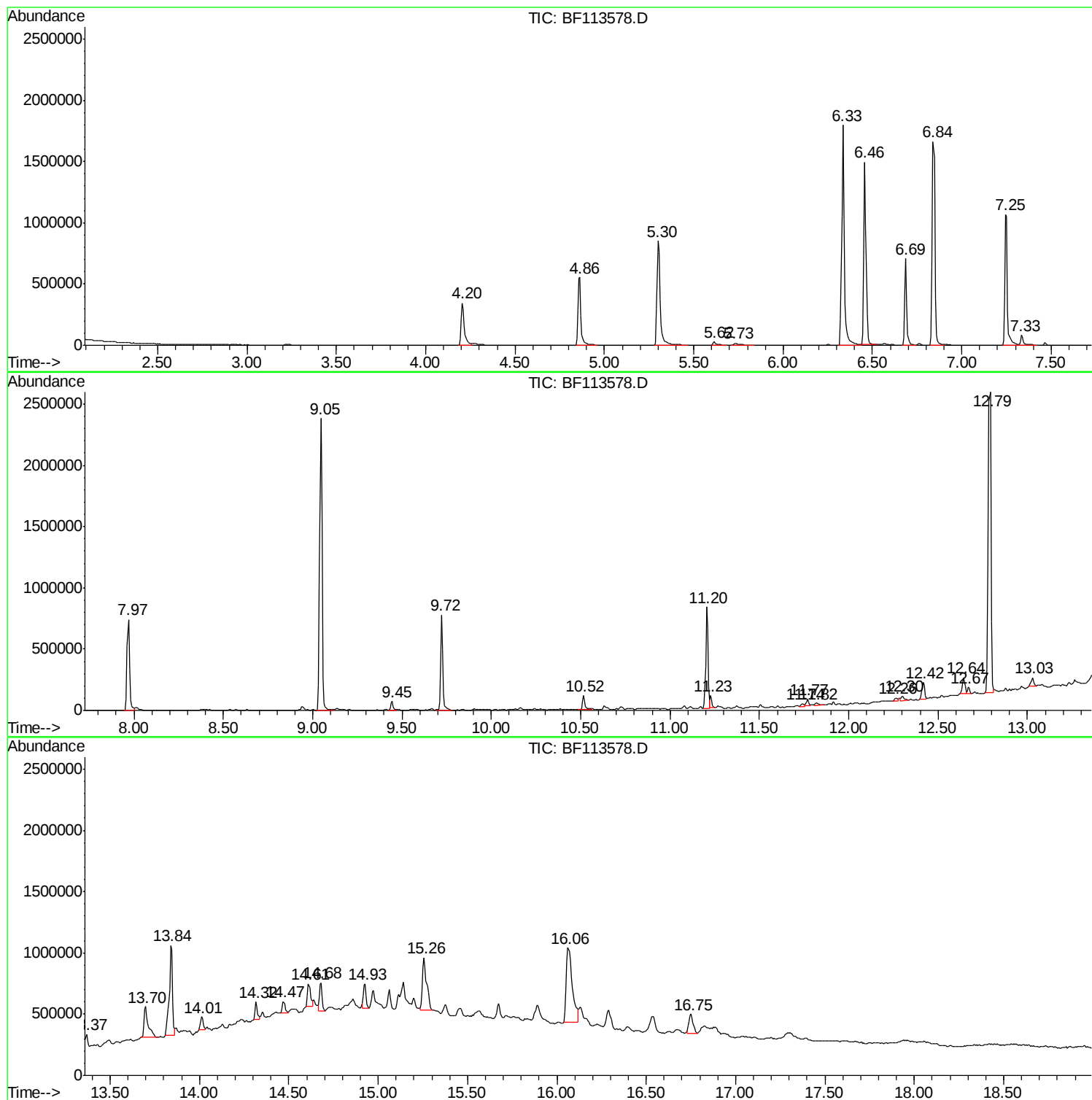
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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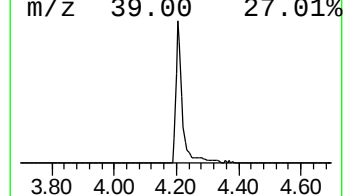
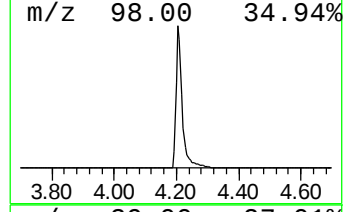
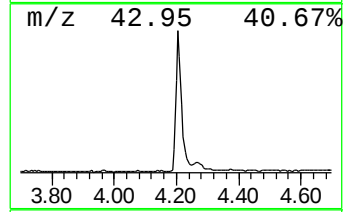
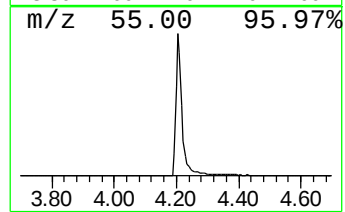
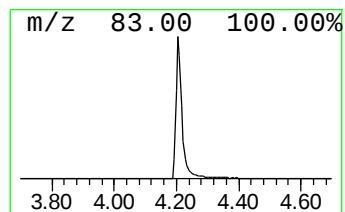
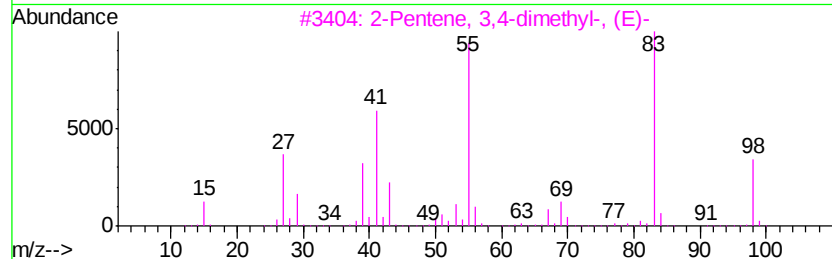
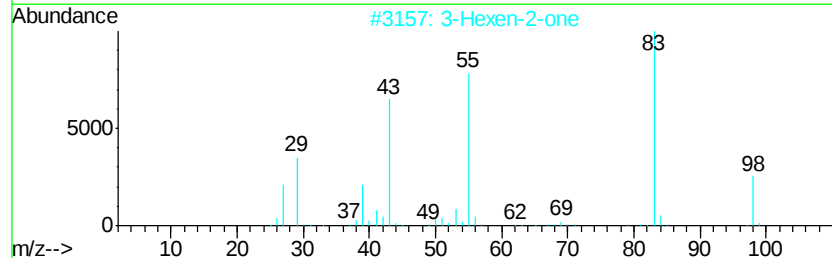
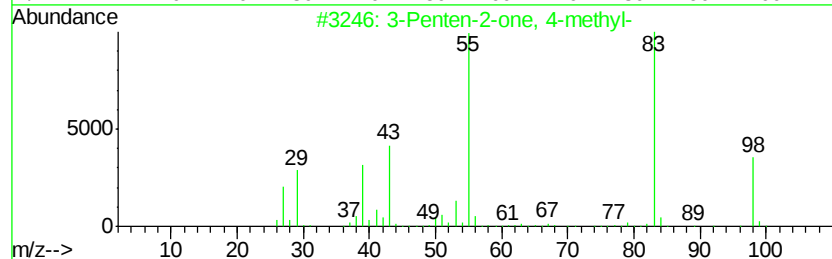
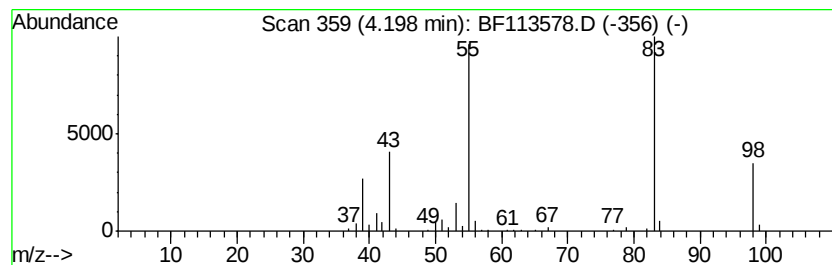
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.20	15.55 ng	457945	1,4-Dichlorobenzene-d4	6.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
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, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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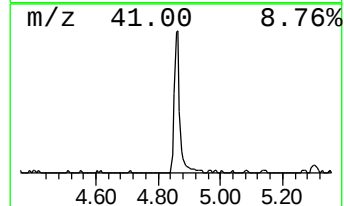
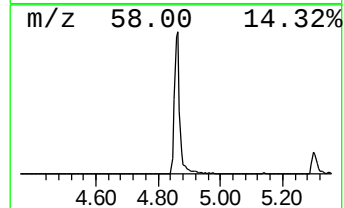
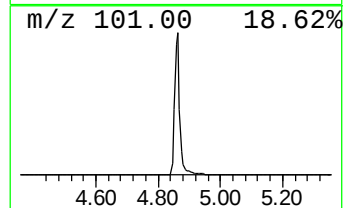
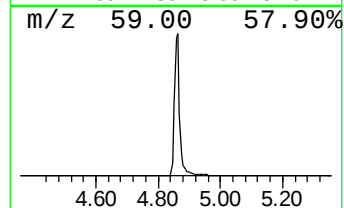
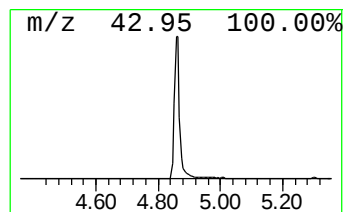
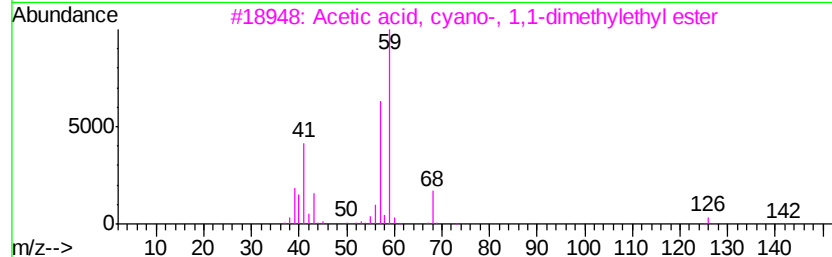
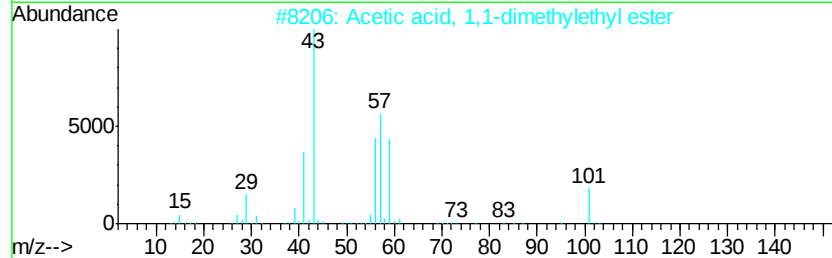
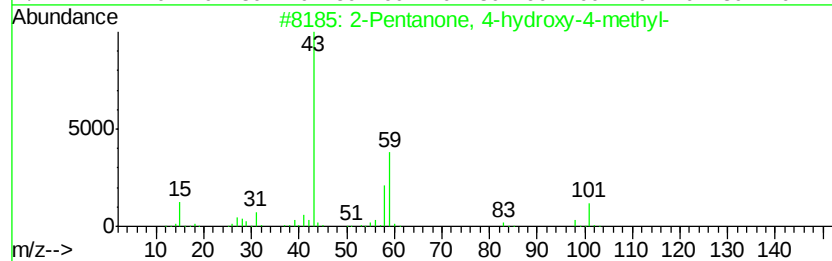
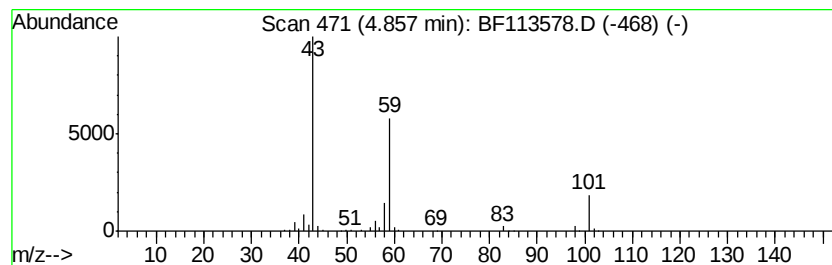
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	23.05 ng	678960	1,4-Dichlorobenzene-d4	6.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
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	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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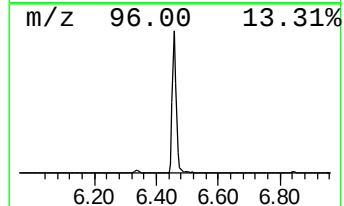
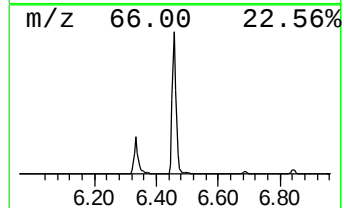
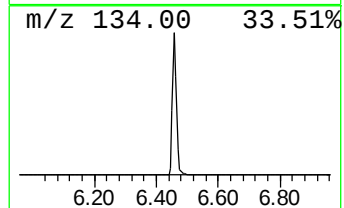
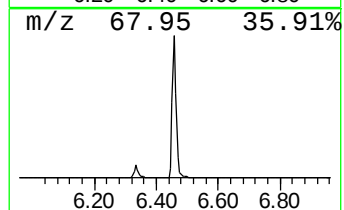
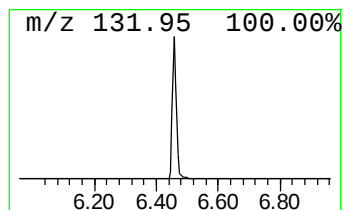
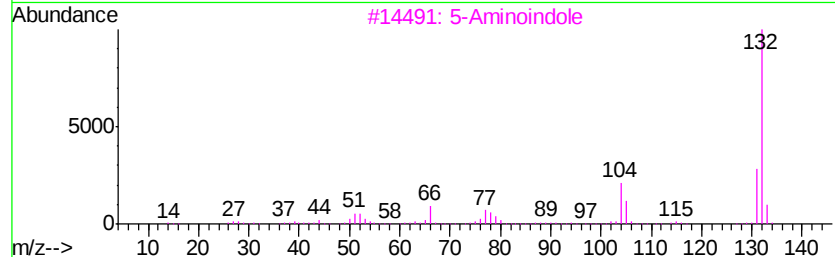
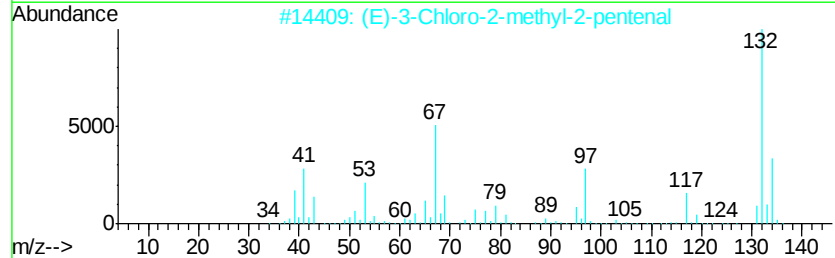
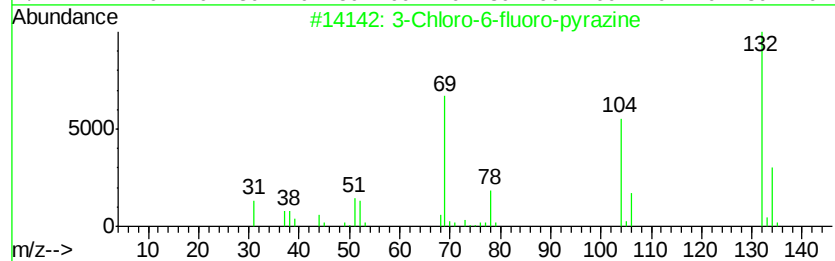
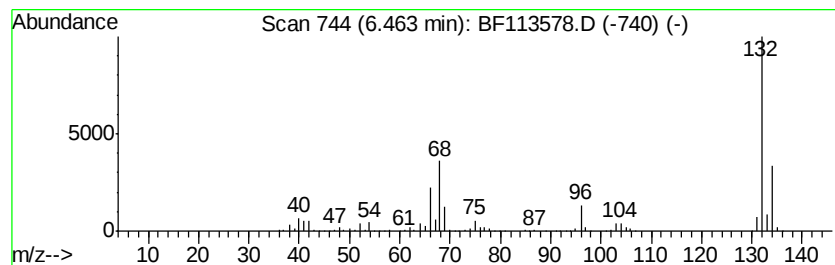
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.46 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	43.26 ng	1274350	1,4-Dichlorobenzene-d4	6.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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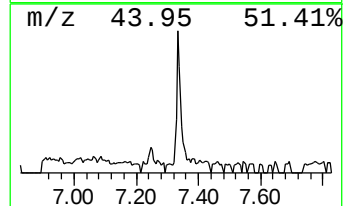
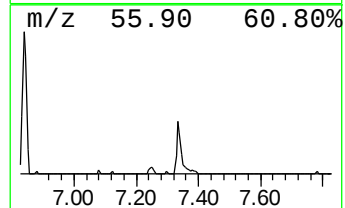
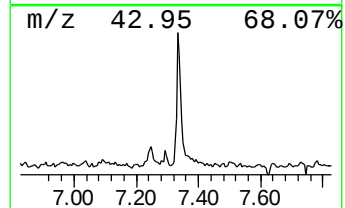
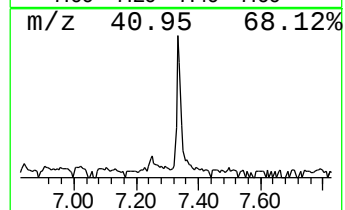
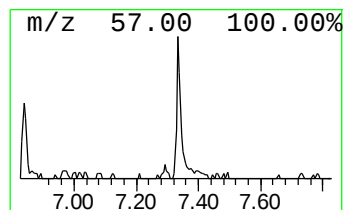
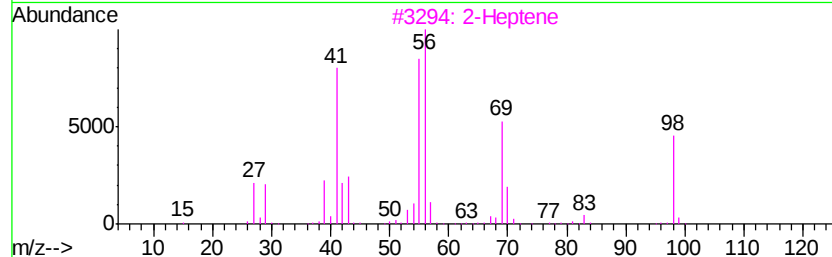
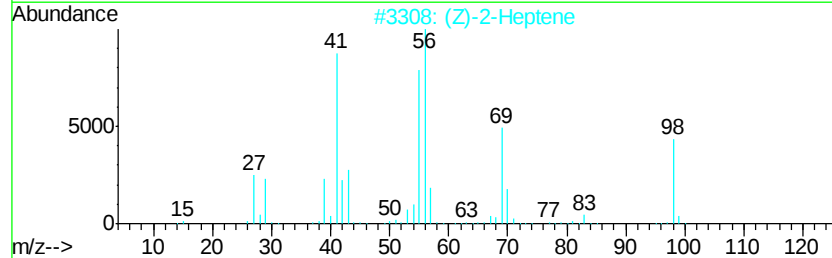
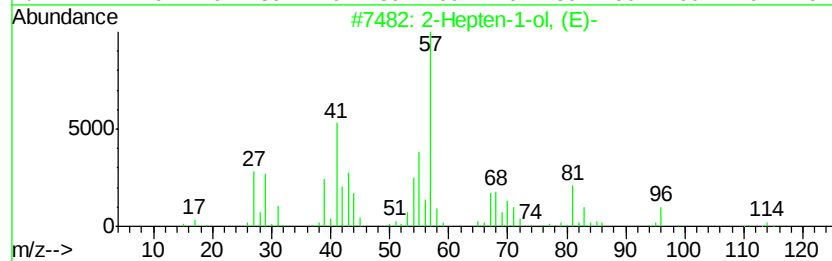
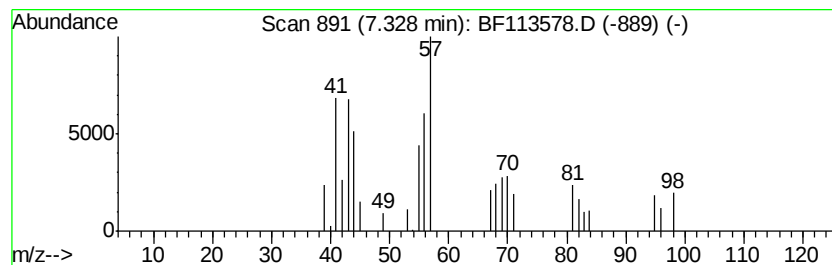
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown7.33 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.33	2.75 ng	90338	Naphthalene-d8	7.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hepten-1-ol, (E)-	114	C7H14O	033467-76-4	43
2		(Z)-2-Heptene	98	C7H14	006443-92-1	30
3		2-Heptene	98	C7H14	000592-77-8	30
4		2-Heptene, (E)-	98	C7H14	014686-13-6	30
5		Butane, 1-isocyanato-	99	C5H9NO	000111-36-4	27



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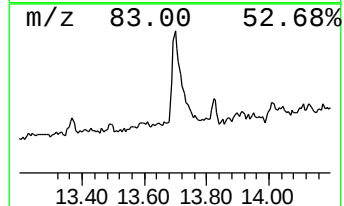
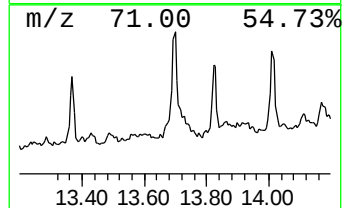
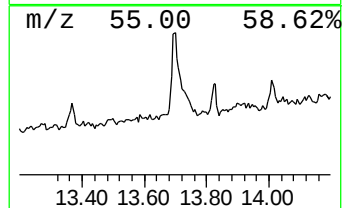
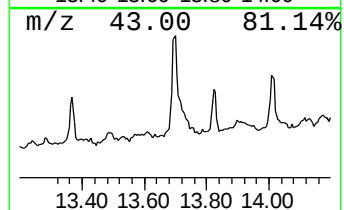
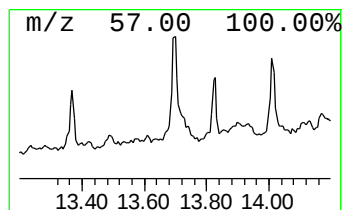
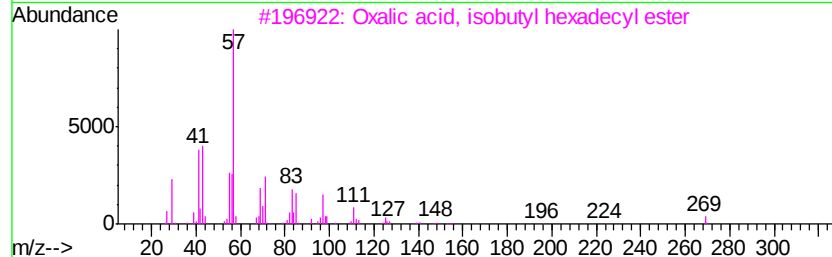
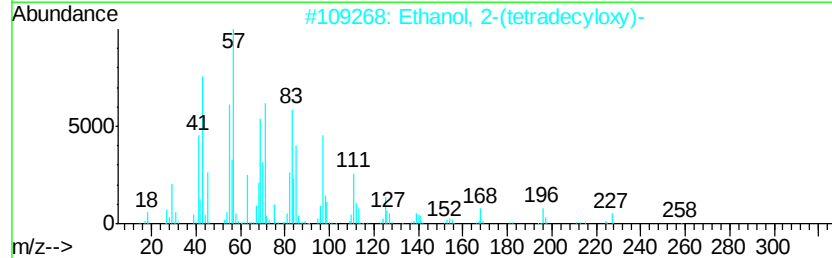
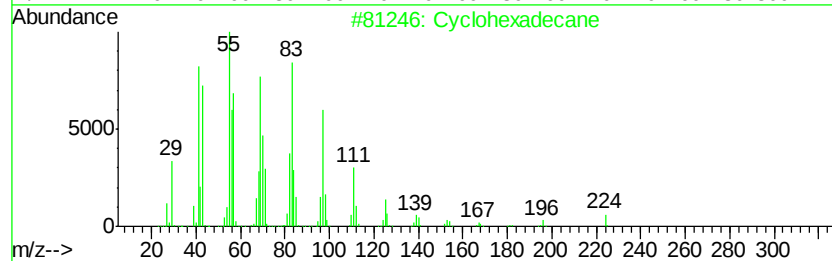
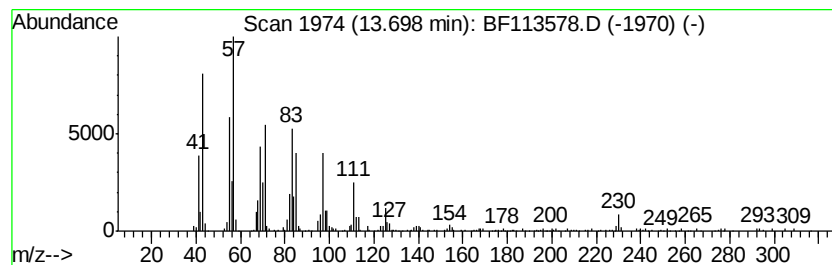
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclohexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	9.09 ng	442041	Chrysene-d12	13.84
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexadecane	224 C16H32	000295-65-8 91
2		Ethanol, 2-(tetradecyloxy)-	258 C16H34O2	002136-70-1 91
3		Oxalic acid, isobutyl hexadecyl ...	370 C22H42O4	1000309-38-1 91
4		Oxalic acid, isobutyl pentadecyl...	356 C21H40O4	1000309-38-0 91
5		5-Octadecene, (E)-	252 C18H36	007206-21-5 90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
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Acq On : 4 Apr 2019 8:41
Operator : JU/SJ
Sample : K2231-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RICH-REC-ROAD-STONE-13

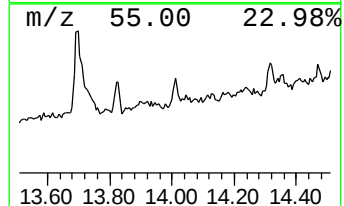
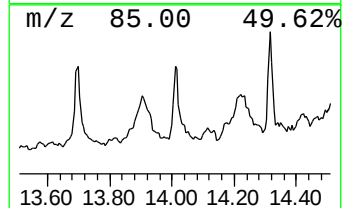
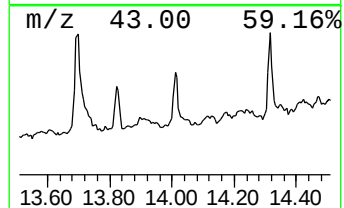
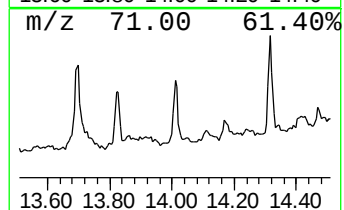
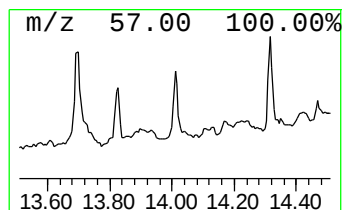
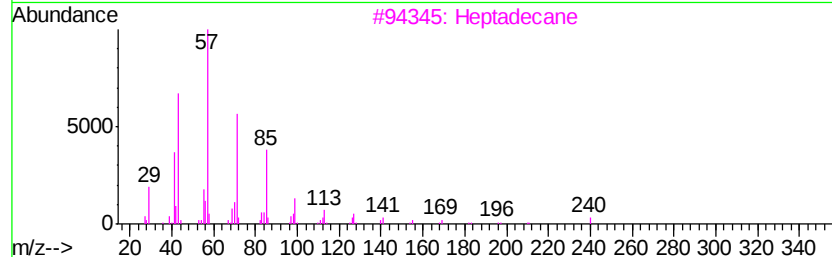
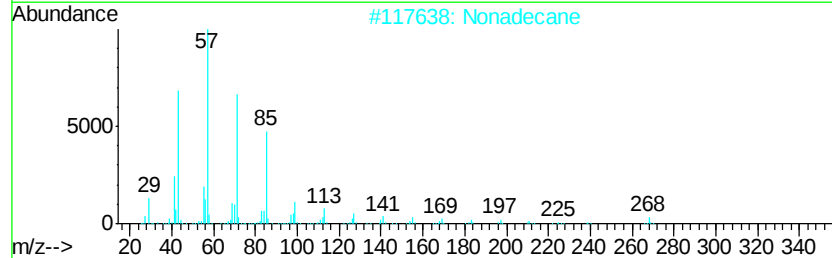
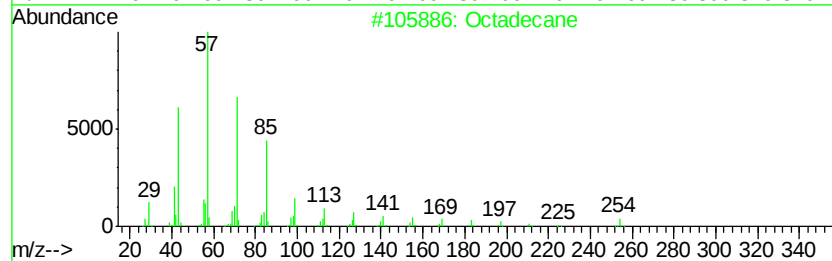
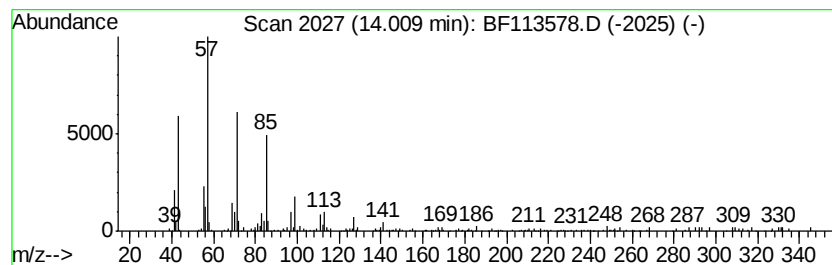
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.01	2.12 ng	103049	Chrysene-d12	13.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	90
2		Nonadecane	268	C19H40	000629-92-5	90
3		Heptadecane	240	C17H36	000629-78-7	87
4		Heneicosane	296	C21H44	000629-94-7	87
5		Hexacosane	366	C26H54	000630-01-3	87



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ClientSampleId :
RICH-REC-ROAD-STONE-13

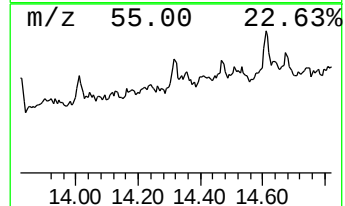
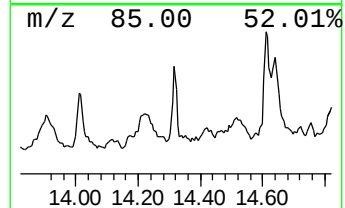
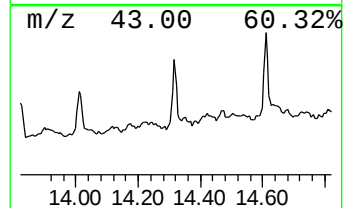
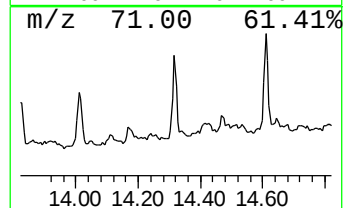
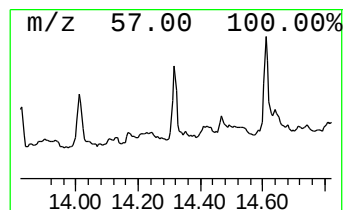
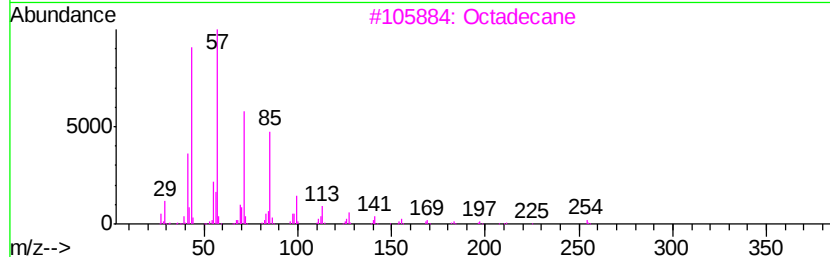
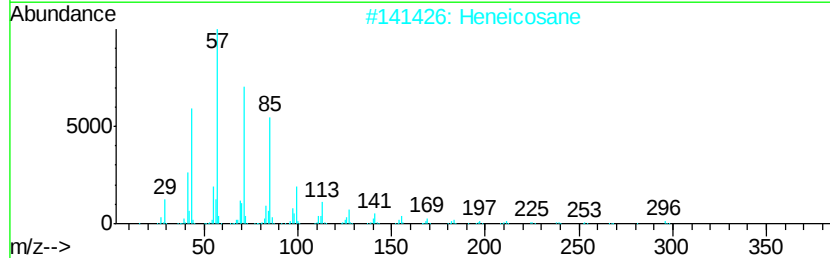
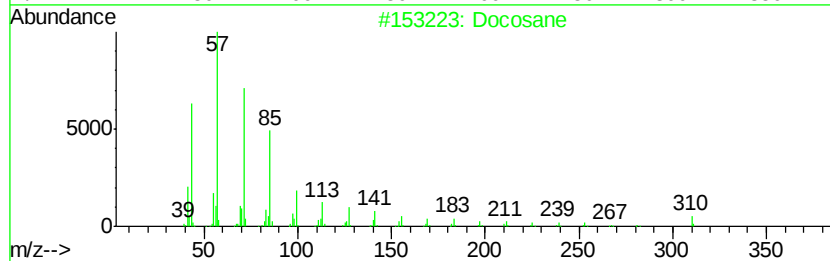
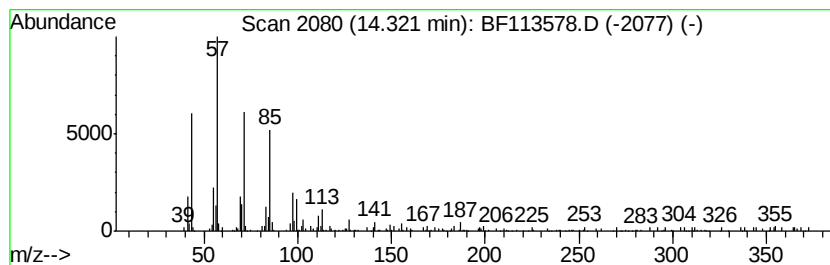
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Docosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	2.69 ng	130880	Chrysene-d12	13.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane	310	C22H46	000629-97-0	93
2		Heneicosane	296	C21H44	000629-94-7	87
3		Octadecane	254	C18H38	000593-45-3	86
4		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
5		Hexadecane	226	C16H34	000544-76-3	78



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
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Sample : K2231-01
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ClientSampleId :
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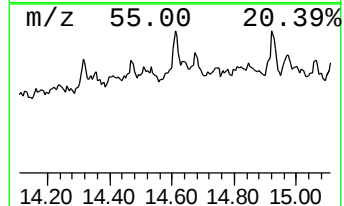
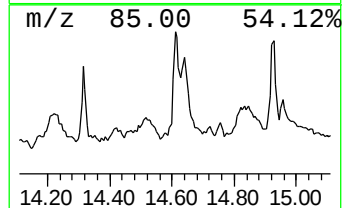
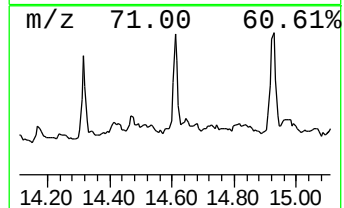
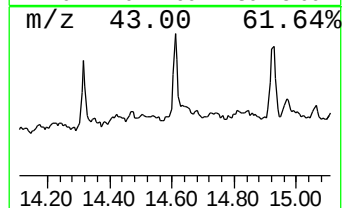
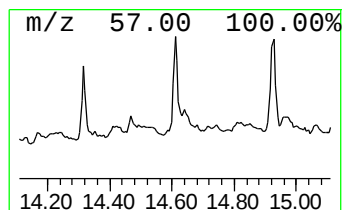
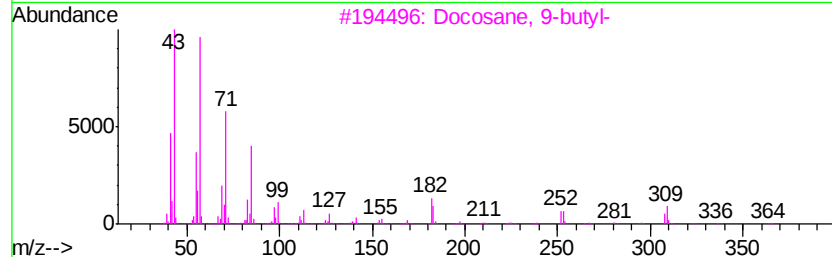
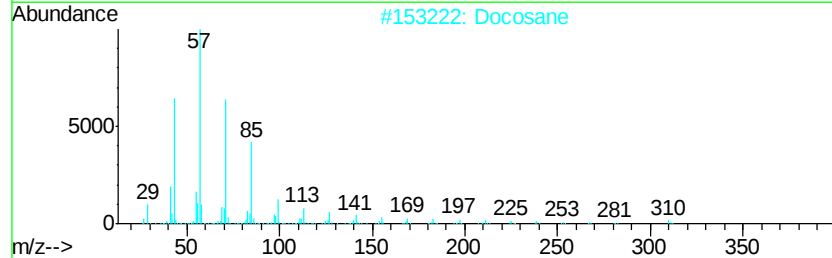
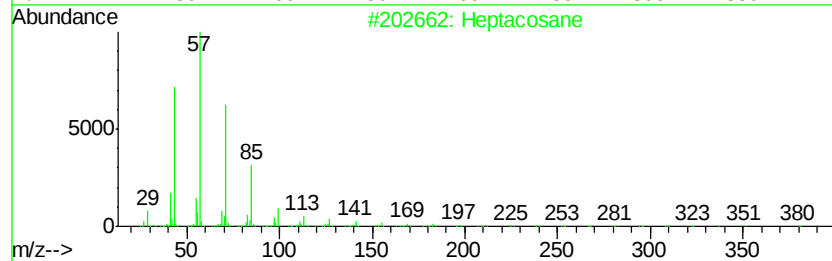
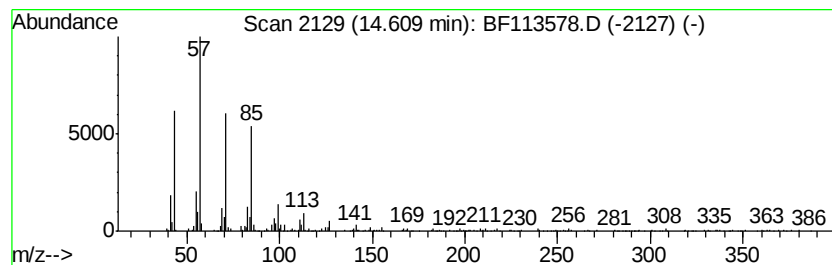
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	5.68 ng	206526	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	90
2		Docosane	310	C22H46	000629-97-0	86
3		Docosane, 9-butyl-	366	C26H54	055282-14-9	86
4		Pentadecane	212	C15H32	000629-62-9	86
5		Heneicosane	296	C21H44	000629-94-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
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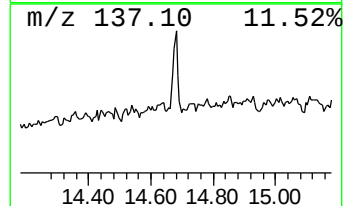
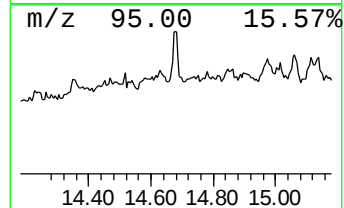
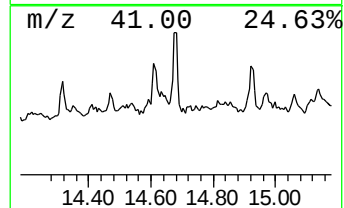
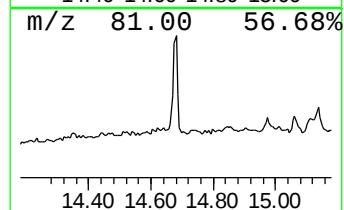
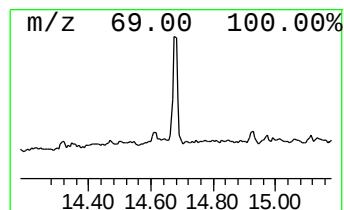
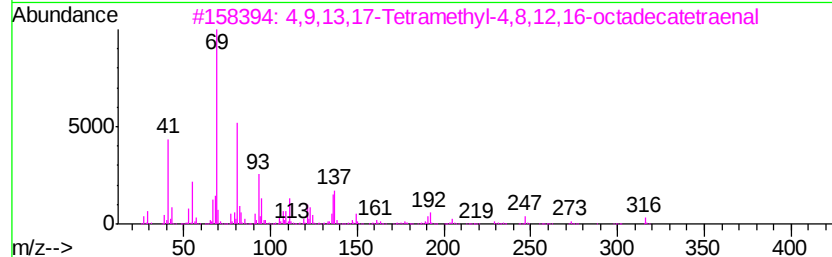
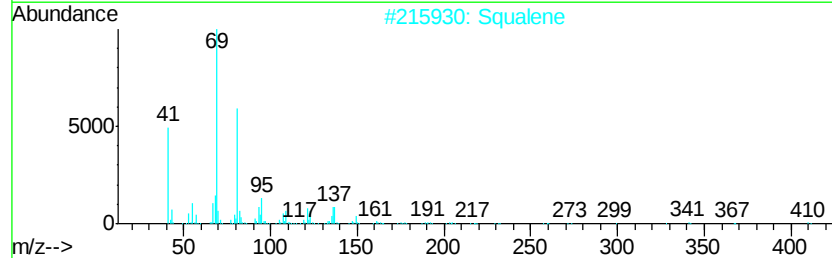
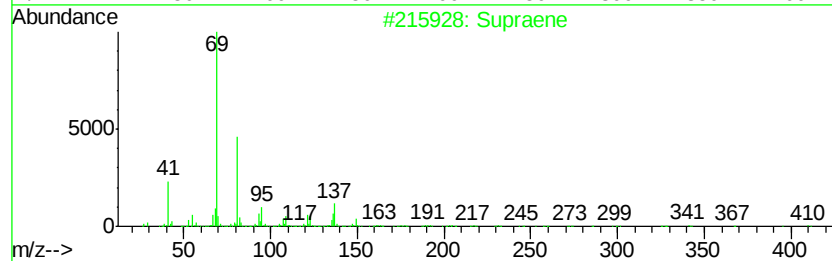
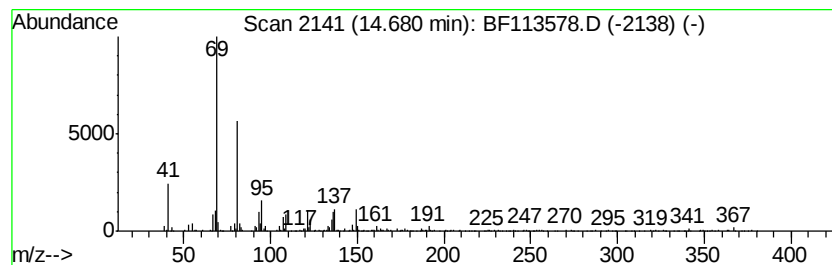
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 10 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.68	6.88 ng	249928	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	86
2		Squalene	410	C30H50	000111-02-4	80
3		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H360	056882-09-8	72
4		1,6-Octadien-3-ol, 3,7-dimethyl-...	182	C11H1802	000115-99-1	53
5		2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
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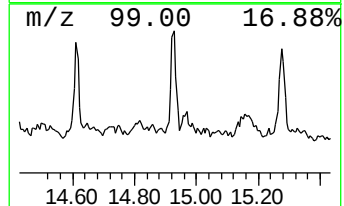
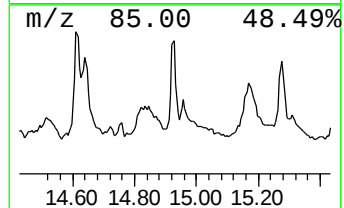
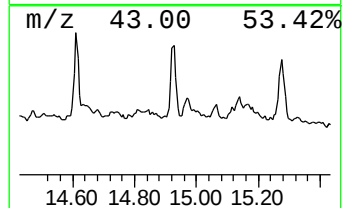
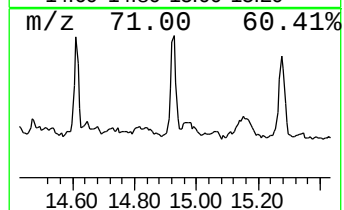
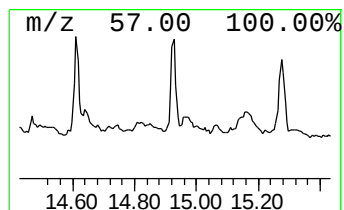
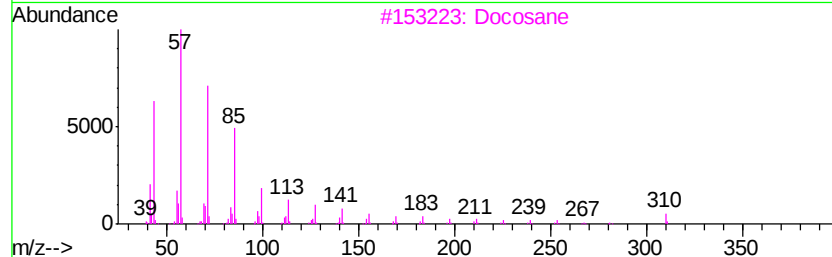
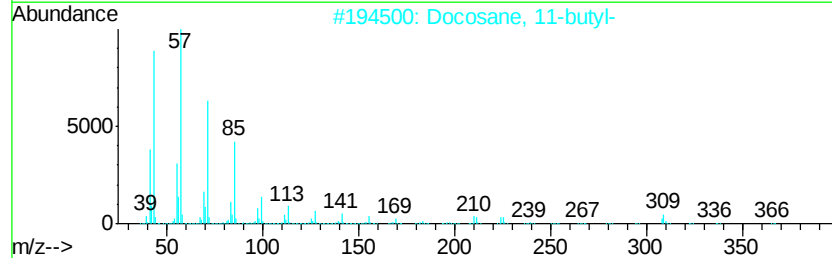
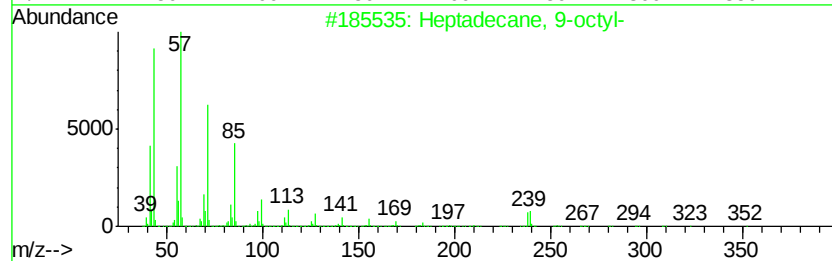
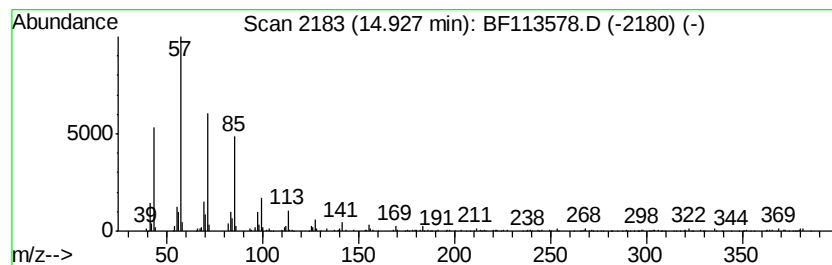
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Heptadecane, 9-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	5.99 ng	217499	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
2		Docosane, 11-butyl-	366	C26H54	013475-76-8	86
3		Docosane	310	C22H46	000629-97-0	86
4		Octadecane, 2-methyl-	268	C19H40	001560-88-9	86
5		Octacosane	394	C28H58	000630-02-4	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
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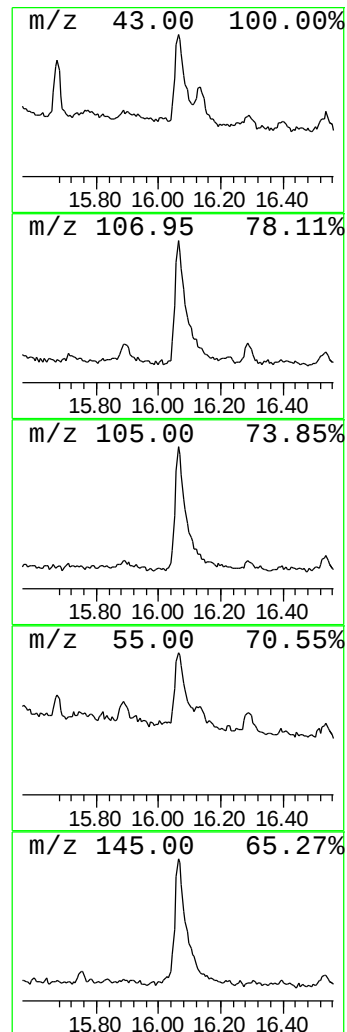
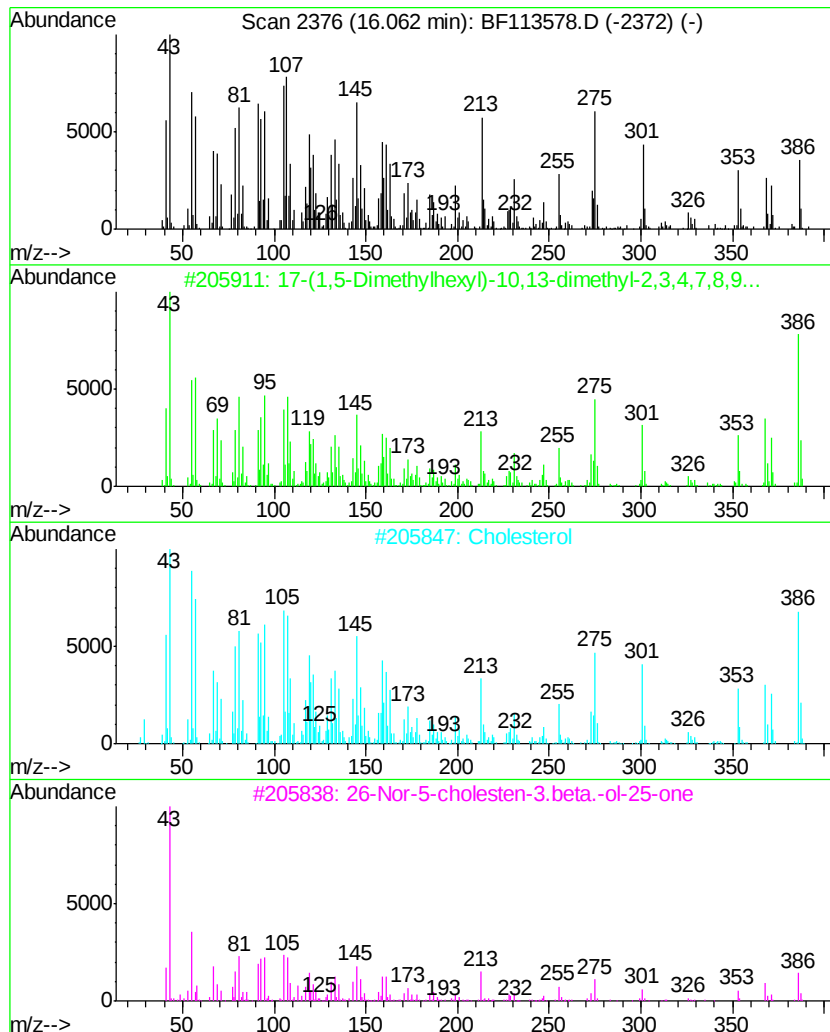
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TIC Integration Parameters: LSCINT.P

Peak Number 12 17-(1,5-Dimethylhexyl)-10,1... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.06	38.56 ng	1400940	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	17-(1,5-Dimethylhexyl)-10,13-dim...	386	C27H46O	1000210-38-4	99
2		Cholesterol	386	C27H46O	000057-88-5	99
3		26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	99
4		Cholestane-3,5-diol, 5-acetate, ...	446	C29H50O3	041721-93-1	64
5		Guaia-1(10),11-diene	204	C15H24	1000374-19-7	22



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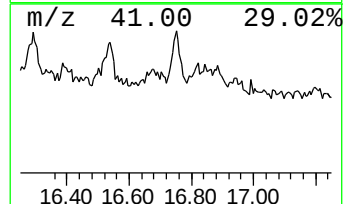
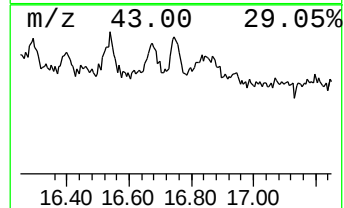
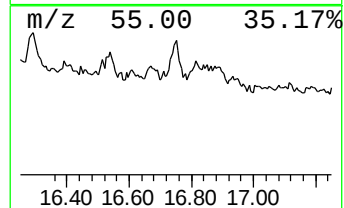
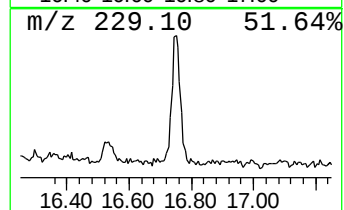
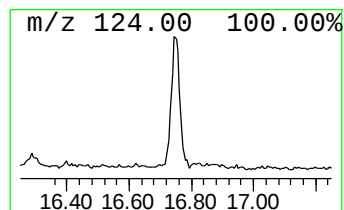
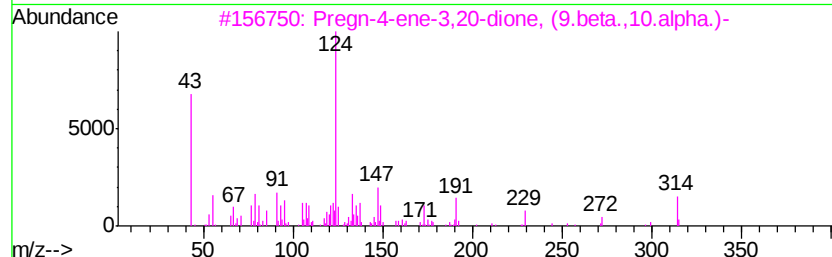
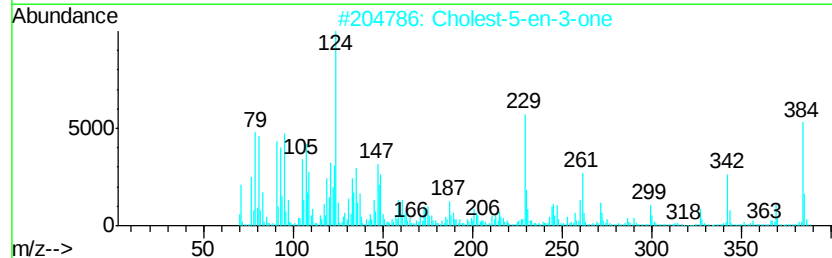
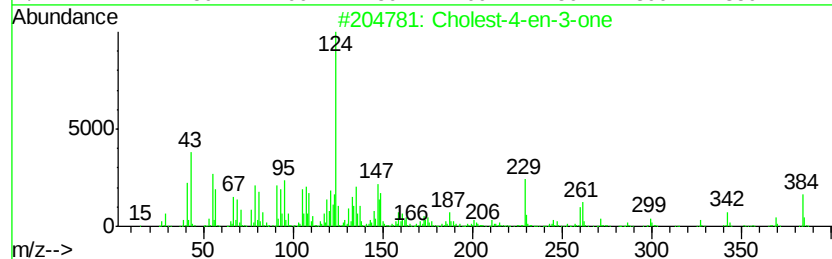
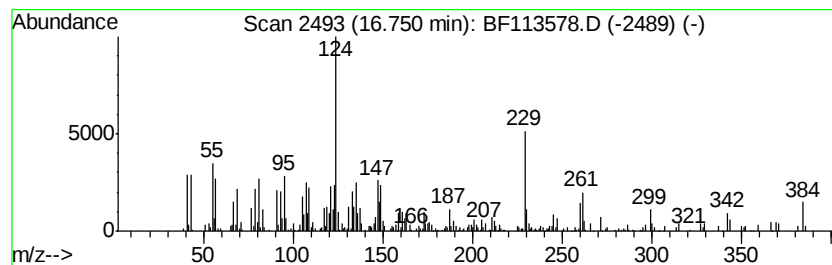
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Cholest-4-en-3-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.75	7.07 ng	256783	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cholest-4-en-3-one	384	C27H44O	000601-57-0	95
2		Cholest-5-en-3-one	384	C27H44O	000601-54-7	92
3		Pregn-4-ene-3,20-dione, (9.beta....	314	C21H30O2	002755-10-4	38
4		Tetralin, 6-acetyl-8-isopropyl-2...	244	C17H24O	1000155-43-5	25
5		Benzenemethanol, 3-hydroxy-	124	C7H8O2	000620-24-6	18



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 Sample : K2231-01
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RICH-REC-ROAD-STONE-13

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.20	15.6	ng	457945	1	6.69	589169	20.0
2-Pentanone, 4-hy...	4.86	23.1	ng	678960	1	6.69	589169	20.0
unknown6.46	6.46	43.3	ng	1274350	1	6.69	589169	20.0
unknown7.33	7.33	2.8	ng	90338	2	7.97	657233	20.0
Cyclohexadecane	13.70	9.1	ng	442041	5	13.84	972228	20.0
Octadecane	14.01	2.1	ng	103049	5	13.84	972228	20.0
Docosane	14.32	2.7	ng	130880	5	13.84	972228	20.0
Heptacosane	14.61	5.7	ng	206526	6	15.26	726632	20.0
Supraene	14.68	6.9	ng	249928	6	15.26	726632	20.0
Heptadecane, 9-oc...	14.93	6.0	ng	217499	6	15.26	726632	20.0
17-(1,5-Dimethylh...	16.06	38.6	ng	1400940	6	15.26	726632	20.0
Cholest-4-en-3-one	16.75	7.1	ng	256783	6	15.26	726632	20.0