LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109680.D
Acq On : 9 Oct 2018 7:01
Operator : JU/SJ
Sample : J5305-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 331-CON

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-BF100818.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	4.245	363	367	390	rBV	316095	501336	37.28%	3.756%
2	4.887	472	476	492	rBV	322610	375187	27.90%	2.811%
3	5.322	547	550	575	rBV	425605	658951	49.01%	4.937%
4	6.345	721	724	741	rBV	607846	969788	72.12%	7.265%
5	6.469	741	745	770	rVB	804778	1020408	75.89%	7.645%
6	6.698	780	784	806	rVB	380043	520685	38.72%	3.901%
7	6.851	806	810	828	rBV	894268	935810	69.59%	7.011%
8	7.257	876	879	912	rBV	466272	758056	56.38%	5.679%
9	7.975	998	1001	1030	rBV	501355	665697	49.51%	4.987%
10	9.051	1180	1184	1210	rBV	1265410	1344658	100.00%	10.074%
11	9.445	1248	1251	1259	rBV	30371	34739	2.58%	0.260%
12	9.722	1294	1298	1312	rBV	607025	646510	48.08%	4.844%
13	10.510	1429	1432	1448	rBV	121412	174870	13.00%	1.310%
14	10.621	1448	1451	1454	rBV	47175	40110	2.98%	0.300%
15	11.204	1546	1550	1560	rBV2	474709	624301	46.43%	4.677%
16	11.280	1560	1563	1571	rVB	15543	26733	1.99%	0.200%
17	11.733	1637	1640	1646	rBV4	13977	21352	1.59%	0.160%
18	11.816	1651	1654	1662	rVB	25426	38051	2.83%	0.285%
19	12.339	1739	1743	1746	rBV	13207	15655	1.16%	0.117%
20	12.410	1751	1755	1761	rBV	190116	216565	16.11%	1.622%
21	12.633	1788	1793	1797	rBV	197258	226987	16.88%	1.701%
22	12.686	1800	1802	1806	rVB4	15913	18283	1.36%	0.137%
23	12.780	1814	1818	1826	rVV	1110007	1035408	77.00%	7.757%
24	12.851	1827	1830	1837	rVB2	18931	33960	2.53%	0.254%
25	12.945	1842	1846	1847	rBV3	24038	28470	2.12%	0.213%
26	12.963	1847	1849	1853	rVB	24590	27157	2.02%	0.203%
27	13.027	1856	1860	1863	rVV2	19414	26277	1.95%	0.197%
28	13.062	1863	1866	1875	rVB5	22929	36783	2.74%	0.276%
29	13.257	1896	1899	1905	rVB8	8940	16243	1.21%	0.122%
30	13.321	1907	1910	1912	rVV	38894	33940	2.52%	0.254%
31	13.357	1914	1916	1920	rVV3	23614	26180	1.95%	0.196%
32	13.404	1922	1924	1927	rVB	32588	27703	2.06%	0.208%
33	13.474	1933	1936	1939	rBV2	16250	21062	1.57%	0.158%
34	13.580	1951	1954	1957	rBV	28262	34068	2.53%	0.255%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109680.D
Acq On : 9 Oct 2018 7:01
Operator : JU/SJ
Sample : J5305-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 331-CON

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-BF100818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.627	1960	1962	1965	rVV	24879	32418	2.41%	0.243%
36	13.680	1968	1971	1975	rVV	85710	104902	7.80%	0.786%
37	13.710	1975	1976	1981	rVB	30170	20741	1.54%	0.155%
38	13.827	1988	1996	1999	rBV2	629557	807475	60.05%	6.049%
39	13.998	2023	2025	2028	rVB	40136	34244	2.55%	0.257%
40	14.051	2032	2034	2037	rVB4	18156	16422	1.22%	0.123%
41	14.215	2060	2062	2065	rBV	19007	15295	1.14%	0.115%
42	14.304	2074	2077	2080	rBV3	42827	44124	3.28%	0.331%
43	14.592	2123	2126	2130	rBV	49193	50926	3.79%	0.382%
44	14.662	2136	2138	2140	rBV2	15686	18255	1.36%	0.137%
45	14.833	2163	2167	2176	rBV	103165	204668	15.22%	1.533%
46	14.909	2176	2180	2182	rBV	47447	52951	3.94%	0.397%
47	15.109	2211	2214	2219	rVV	36979	48730	3.62%	0.365%
48	15.168	2221	2224	2229	rVB	46296	65202	4.85%	0.488%
49	15.227	2229	2234	2249	rVB	331762	537314	39.96%	4.025%
50	15.651	2302	2306	2313	rBV	39037	57674	4.29%	0.432%
51	16.103	2379	2383	2392	rVB5	30569	54614	4.06%	0.409%

Sum of corrected areas: 13347938

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
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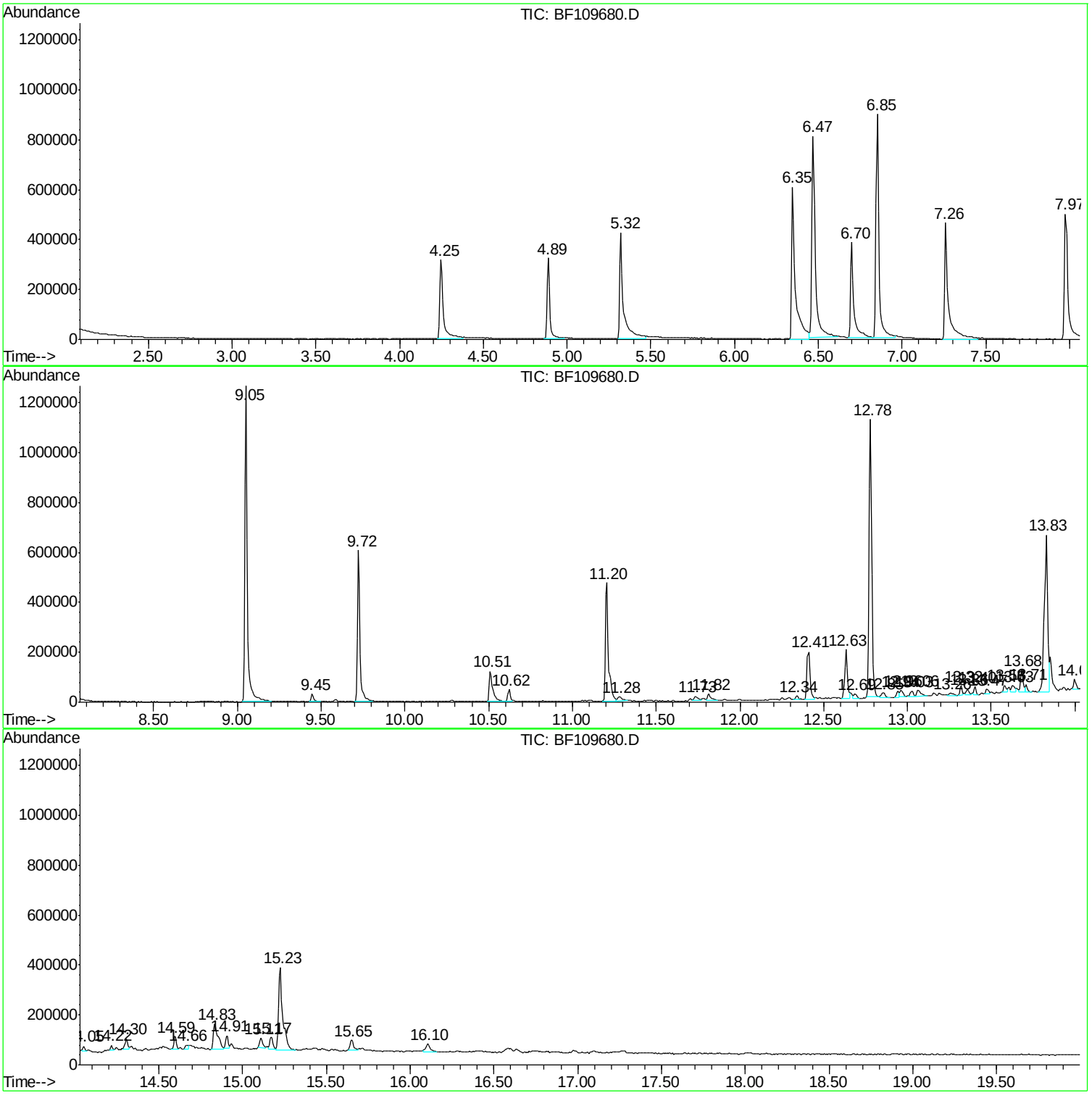
Acq On : 9 Oct 2018 7:01
Operator : JU/SJ
Sample : J5305-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 331-CON

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109680.D
Acq On : 9 Oct 2018 7:01
Operator : JU/SJ
Sample : J5305-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 331-CON

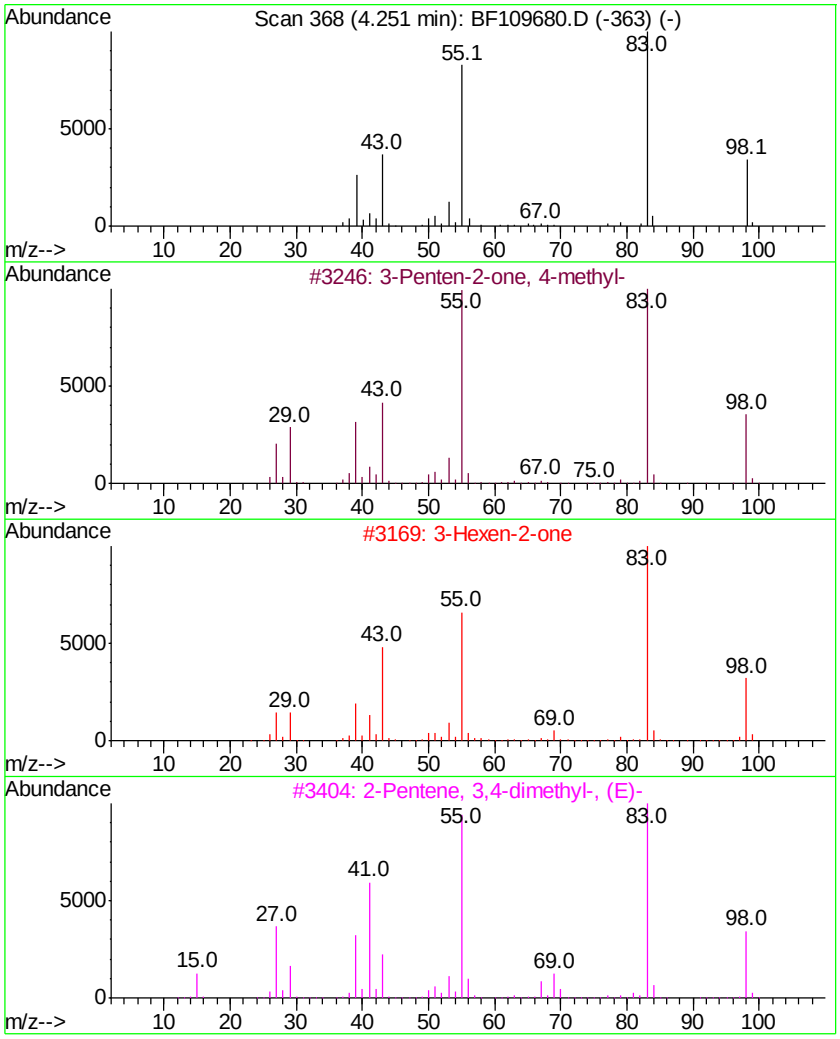
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

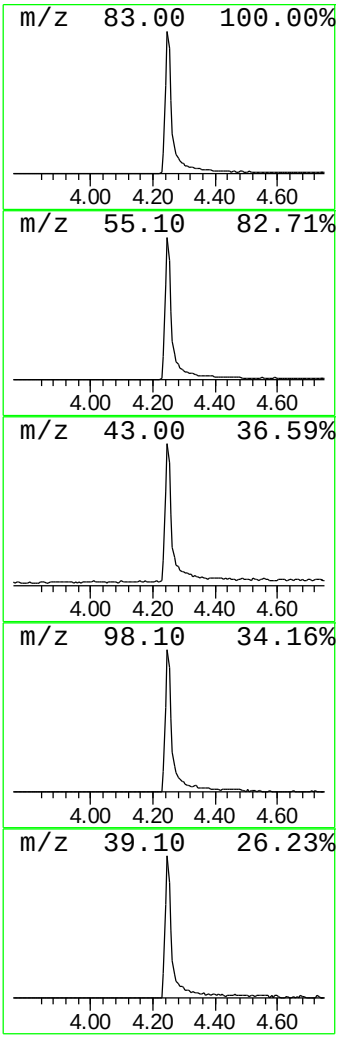
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.25	19.26 ng	501336	1,4-Dichlorobenzene-d4	6.70

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	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109680.D
Acq On : 9 Oct 2018 7:01
Operator : JU/SJ
Sample : J5305-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 331-CON

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

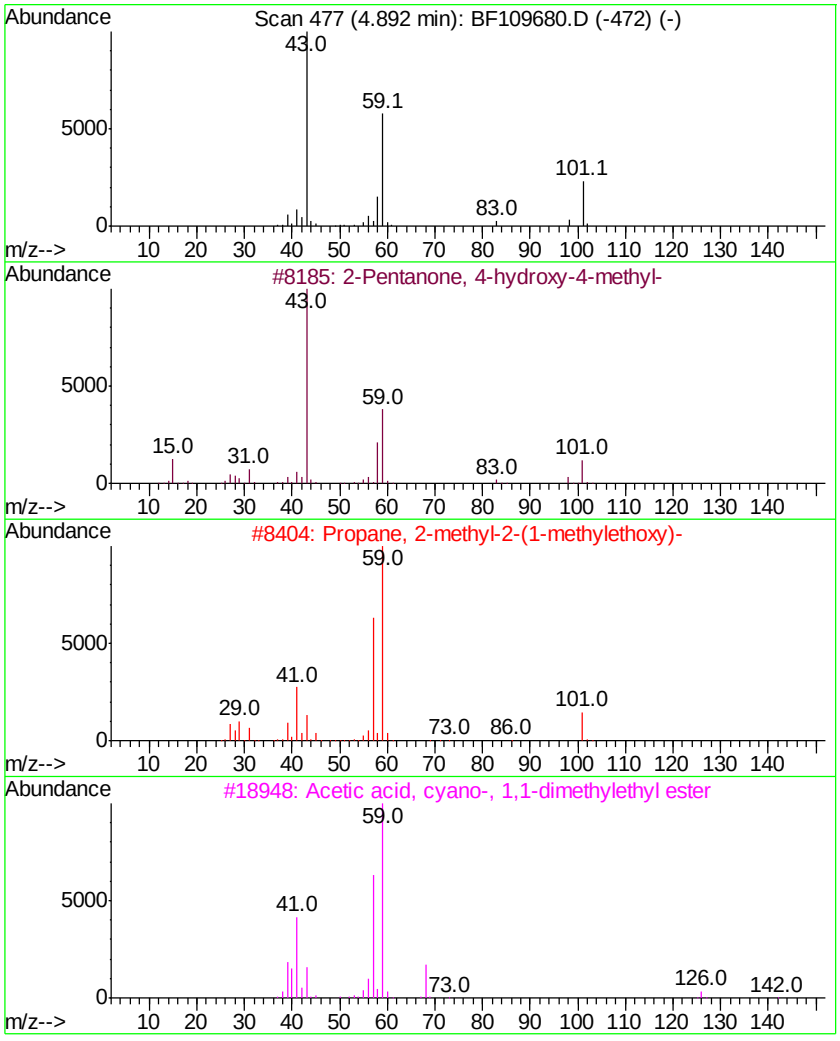
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

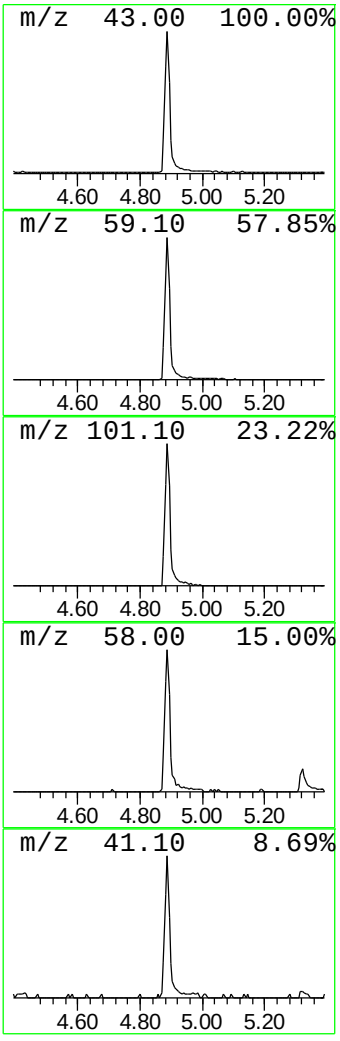
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	14.41 ng	375187	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109680.D
Acq On : 9 Oct 2018 7:01
Operator : JU/SJ
Sample : J5305-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 331-CON

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

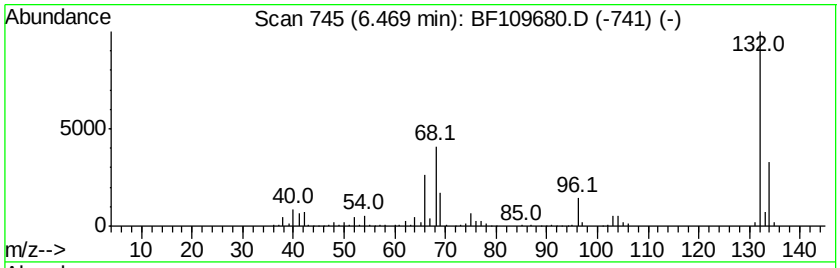
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

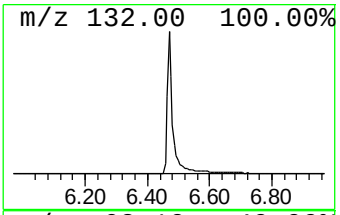
****

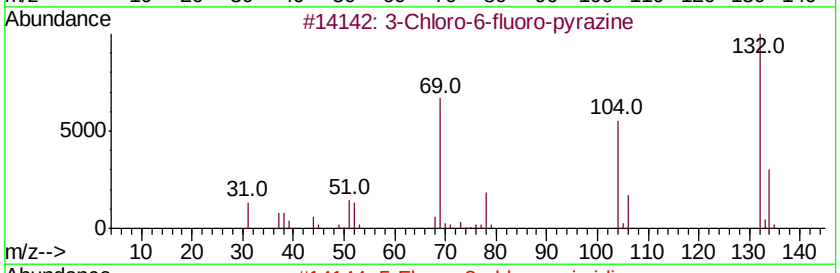
Peak Number 3 unknown6.47 Concentration Rank 1

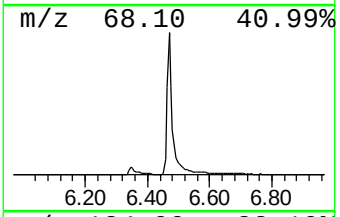
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	39.19 ng	1020410	1,4-Dichlorobenzene-d4	6.70

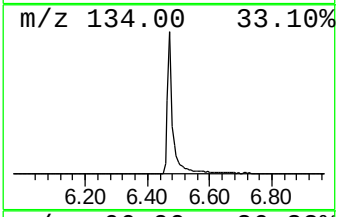
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9

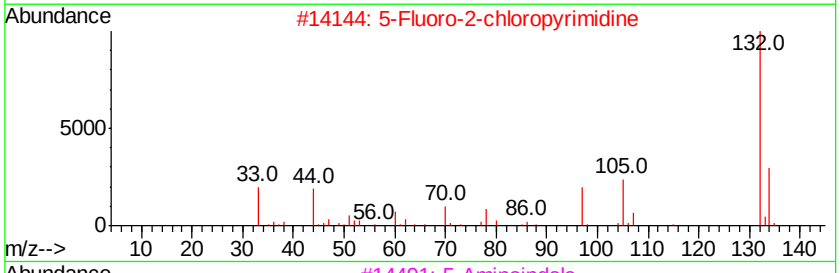


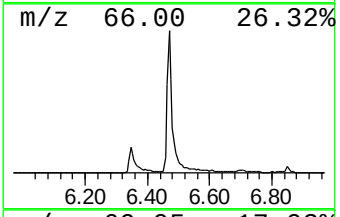


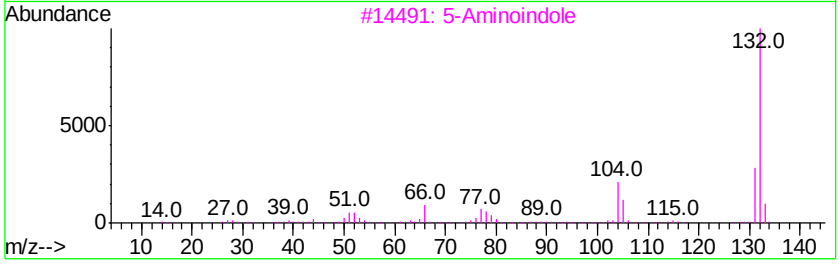


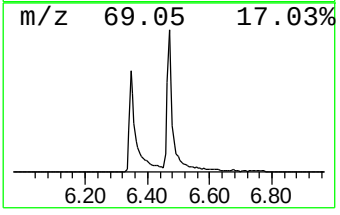












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109680.D
Acq On : 9 Oct 2018 7:01
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Sample : J5305-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 331-CON

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

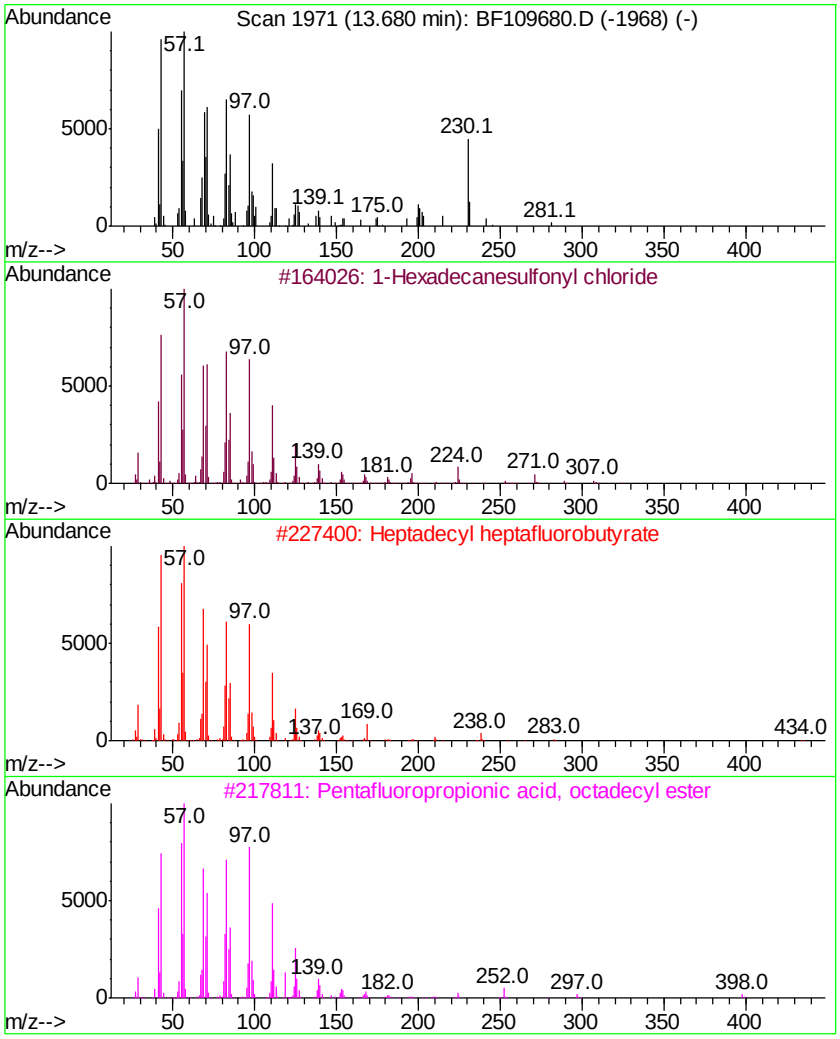
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

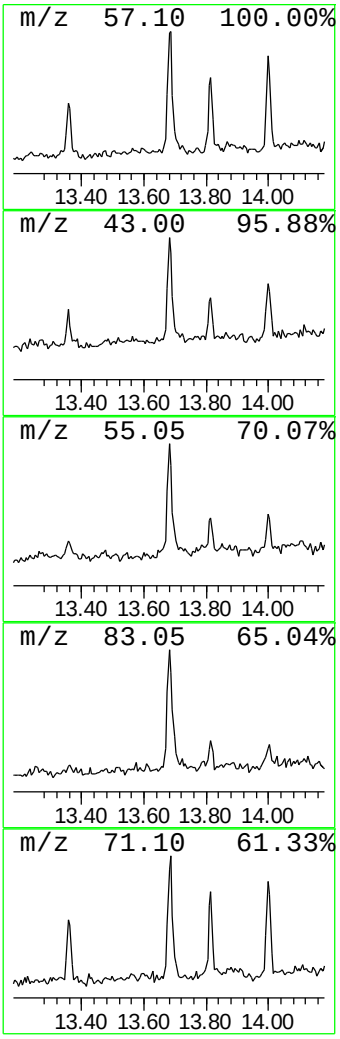
****

Peak Number 5 1-Hexadecanesulfonyl chloride Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	2.60 ng	104902	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	70
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	70
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	62
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	62
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	62





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : 331-CON

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

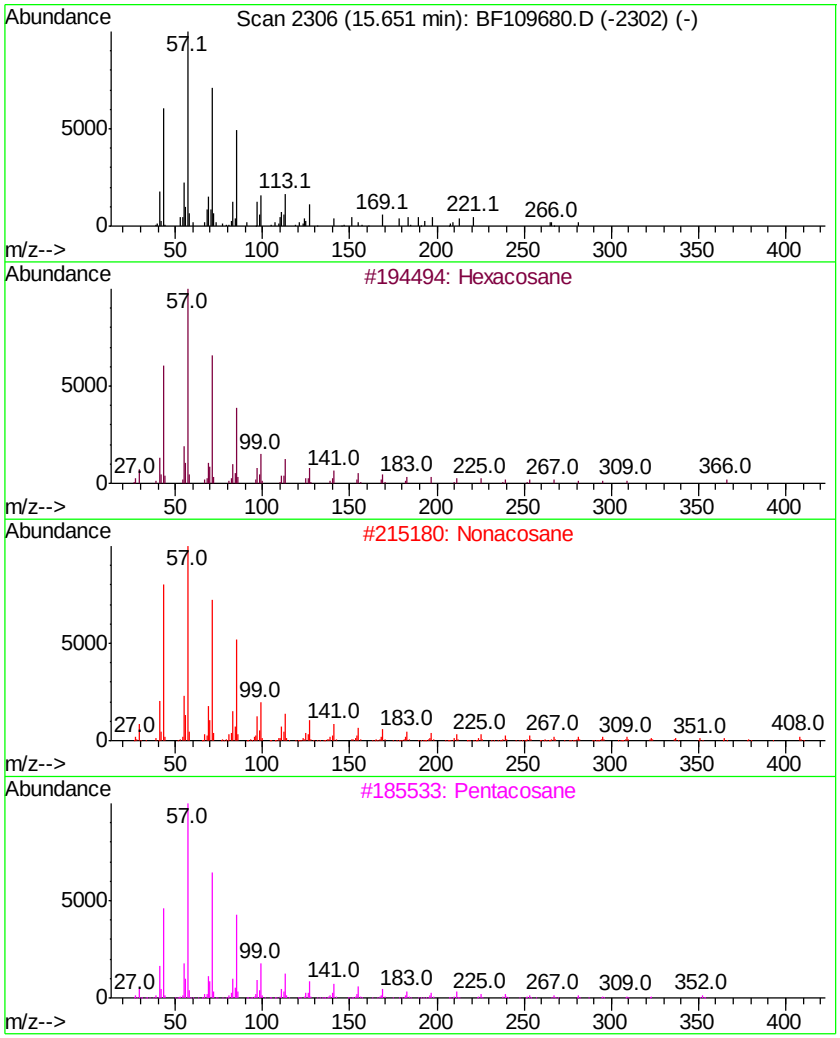
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

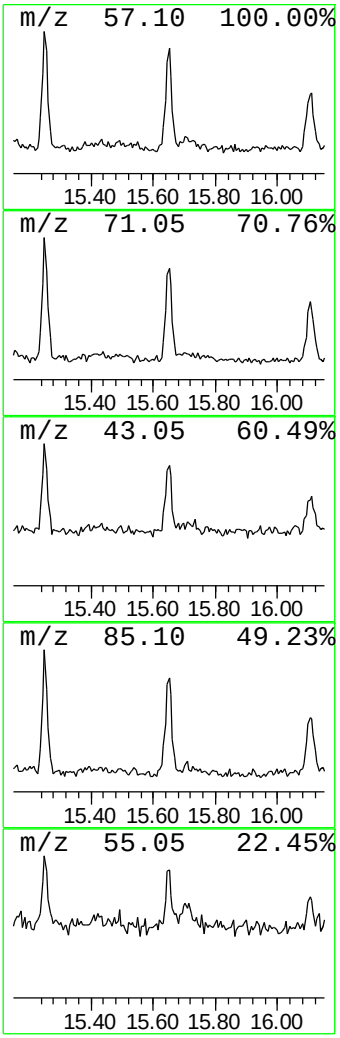
****

Peak Number 6 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.65	2.15 ng	57674	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Nonacosane	408	C29H60	000630-03-5	90
3	Pentacosane	352	C25H52	000629-99-2	90
4	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
5	Octacosane	394	C28H58	000630-02-4	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109680.D
Acq On : 9 Oct 2018 7:01
Operator : JU/SJ
Sample : J5305-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 331-CON

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

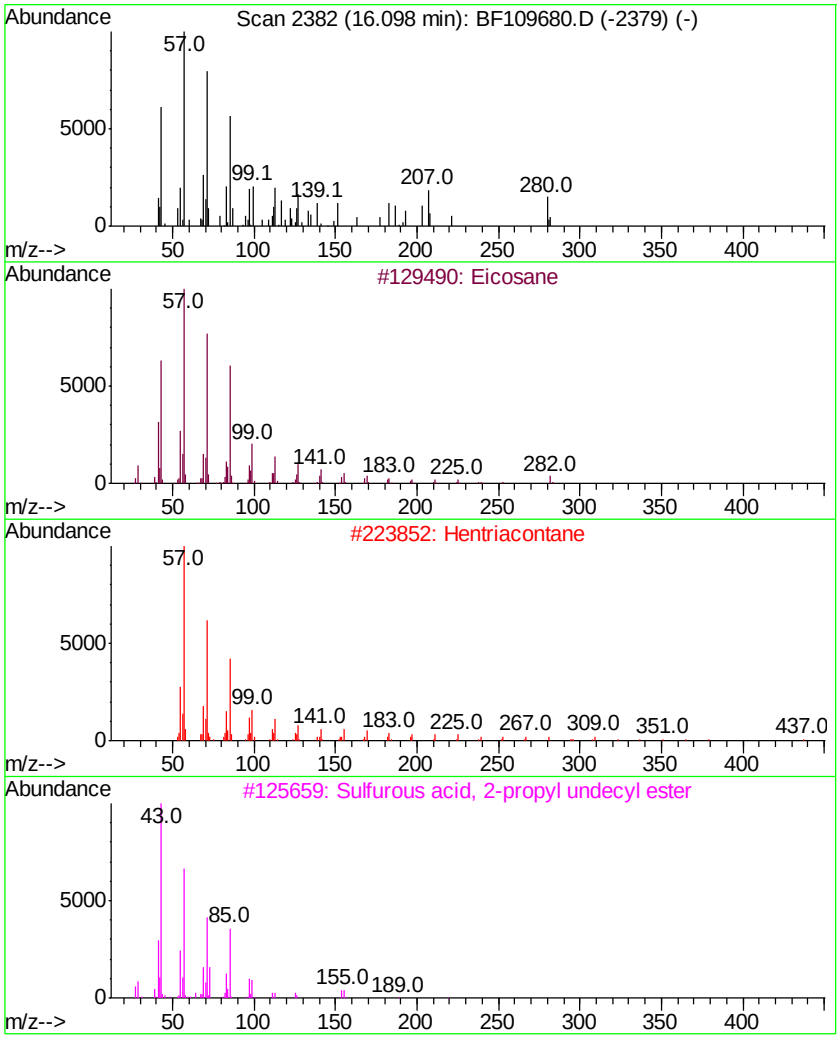
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

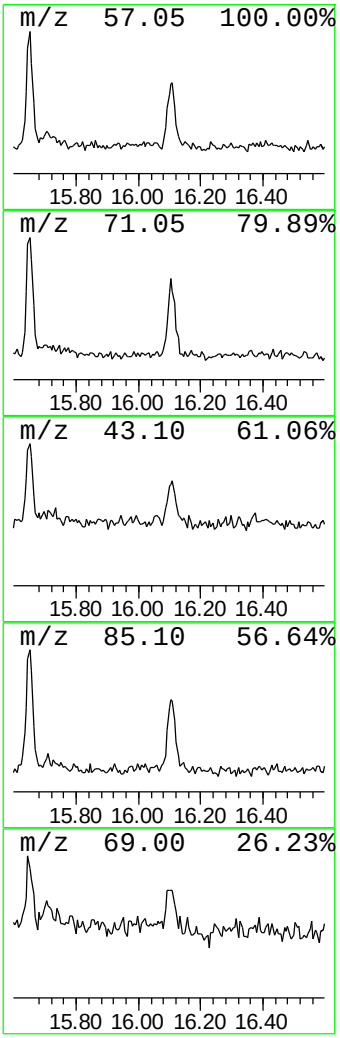
****

Peak Number 7 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	2.03 ng	54614	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Hentriacontane	437	C31H64	000630-04-6	64
3	Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	53
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	53
5	Decane, 1-bromo-2-methyl-	234	C11H23Br	127839-47-8	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100818\
Data File : BF109680.D
Acq On : 9 Oct 2018 7:01
Operator : JU/SJ
Sample : J5305-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 331-CON

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.25	19.3	ng	501336	1	6.70	520685	20.0
2-Pentanone, 4-hy...	4.89	14.4	ng	375187	1	6.70	520685	20.0
unknown6.47	6.47	39.2	ng	1020410	1	6.70	520685	20.0
1-Hexadecanesulfo...	13.68	2.6	ng	104902	5	13.83	807475	20.0
Hexacosane	15.65	2.1	ng	57674	6	15.23	537314	20.0
Eicosane	16.10	2.0	ng	54614	6	15.23	537314	20.0