LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080719\
Data File : BF116057.D
Acq On : 7 Aug 2019 20:14
Operator : HP/JU
Sample : K4154-04 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-4

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-BF073019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF116058.D

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.463	571	574	603	rBV	1059849	1239327	86.54%	6.681%
2	6.128	683	687	690	rBB	34217	31708	2.21%	0.171%
3	6.475	743	746	756	rBV	1217360	1307628	91.31%	7.049%
4	6.545	756	758	763	rVV	31172	43134	3.01%	0.233%
5	6.616	766	770	788	rVB	1462792	1378496	96.26%	7.431%
6	6.840	805	808	818	rBV	889462	854249	59.65%	4.605%
7	6.916	818	821	826	rVB	15622	16548	1.16%	0.089%
8	6.998	831	835	847	rBV	1143283	994168	69.42%	5.359%
9	7.404	900	904	916	rBV	660954	781090	54.54%	4.211%
10	8.122	1023	1026	1047	rBV	1107128	1075282	75.08%	5.796%
11	9.192	1205	1208	1221	rBV	1385414	1432118	100.00%	7.720%
12	9.316	1226	1229	1233	rVB2	13575	17856	1.25%	0.096%
13	9.592	1272	1276	1285	rBV	170652	193722	13.53%	1.044%
14	9.751	1300	1303	1306	rVB2	22272	18518	1.29%	0.100%
15	9.875	1321	1324	1336	rVB	1304839	1180212	82.41%	6.362%
16	10.028	1348	1350	1355	rVB	35050	30282	2.11%	0.163%
17	10.663	1455	1458	1468	rBV	531662	621960	43.43%	3.353%
18	10.792	1474	1480	1486	rVB6	34934	56685	3.96%	0.306%
19	10.845	1486	1489	1491	rBV	63357	58529	4.09%	0.316%
20	10.875	1491	1494	1498	rVV2	59349	92017	6.43%	0.496%
21	10.910	1498	1500	1503	rVV	65658	69219	4.83%	0.373%
22	10.933	1503	1504	1507	rVV	31847	30186	2.11%	0.163%
23	10.975	1507	1511	1513	rVV2	22034	35798	2.50%	0.193%
24	11.022	1516	1519	1523	rVV3	41594	56350	3.93%	0.304%
25	11.063	1523	1526	1531	rVV	62835	81227	5.67%	0.438%
26	11.104	1531	1533	1538	rVB2	31954	32107	2.24%	0.173%
27	11.257	1555	1559	1564	rVB4	15149	20936	1.46%	0.113%
28	11.363	1573	1577	1580	rBV	1059343	992661	69.31%	5.351%
29	11.386	1580	1581	1584	rVV	149206	100364	7.01%	0.541%
30	11.439	1588	1590	1595	rVB	26063	31142	2.17%	0.168%
31	11.604	1614	1618	1624	rBV4	16476	28746	2.01%	0.155%
32	11.886	1664	1666	1674	rVB3	36515	55288	3.86%	0.298%
33	11.980	1679	1682	1685	rBV2	15250	17394	1.21%	0.094%
34	12.445	1758	1761	1765	rVB4	18930	17573	1.23%	0.095%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080719\
Data File : BF116057.D
Acq On : 7 Aug 2019 20:14
Operator : HP/JU
Sample : K4154-04 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-4

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-BF073019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.504	1768	1771	1775	rBV2	13397	18856	1.32%	0.102%
36	12.580	1780	1784	1787	rBV	136812	145461	10.16%	0.784%
37	12.610	1787	1789	1796	rVB4	18043	21121	1.47%	0.114%
38	12.698	1801	1804	1807	rVB4	24017	23109	1.61%	0.125%
39	12.804	1817	1822	1825	rBV2	118025	154475	10.79%	0.833%
40	12.833	1825	1827	1837	rVB3	26686	49887	3.48%	0.269%
41	12.939	1842	1845	1853	rVV	1090544	1006858	70.31%	5.428%
42	13.169	1882	1884	1887	rBV2	16705	17070	1.19%	0.092%
43	13.704	1971	1975	1980	rBV	218601	221021	15.43%	1.191%
44	13.839	1996	1998	1999	rBV	48711	40221	2.81%	0.217%
45	14.004	2022	2026	2035	rVB	1005934	1058553	73.92%	5.706%
46	14.527	2113	2115	2120	rVB	73180	75448	5.27%	0.407%
47	15.092	2208	2211	2219	rVB	245564	324831	22.68%	1.751%
48	15.468	2271	2275	2282	rVB	800648	1040389	72.65%	5.608%
49	15.898	2345	2348	2354	rVB	125157	170320	11.89%	0.918%
50	18.292	2748	2755	2775	rVB3	316656	1190744	83.15%	6.419%

Sum of corrected areas: 18550884

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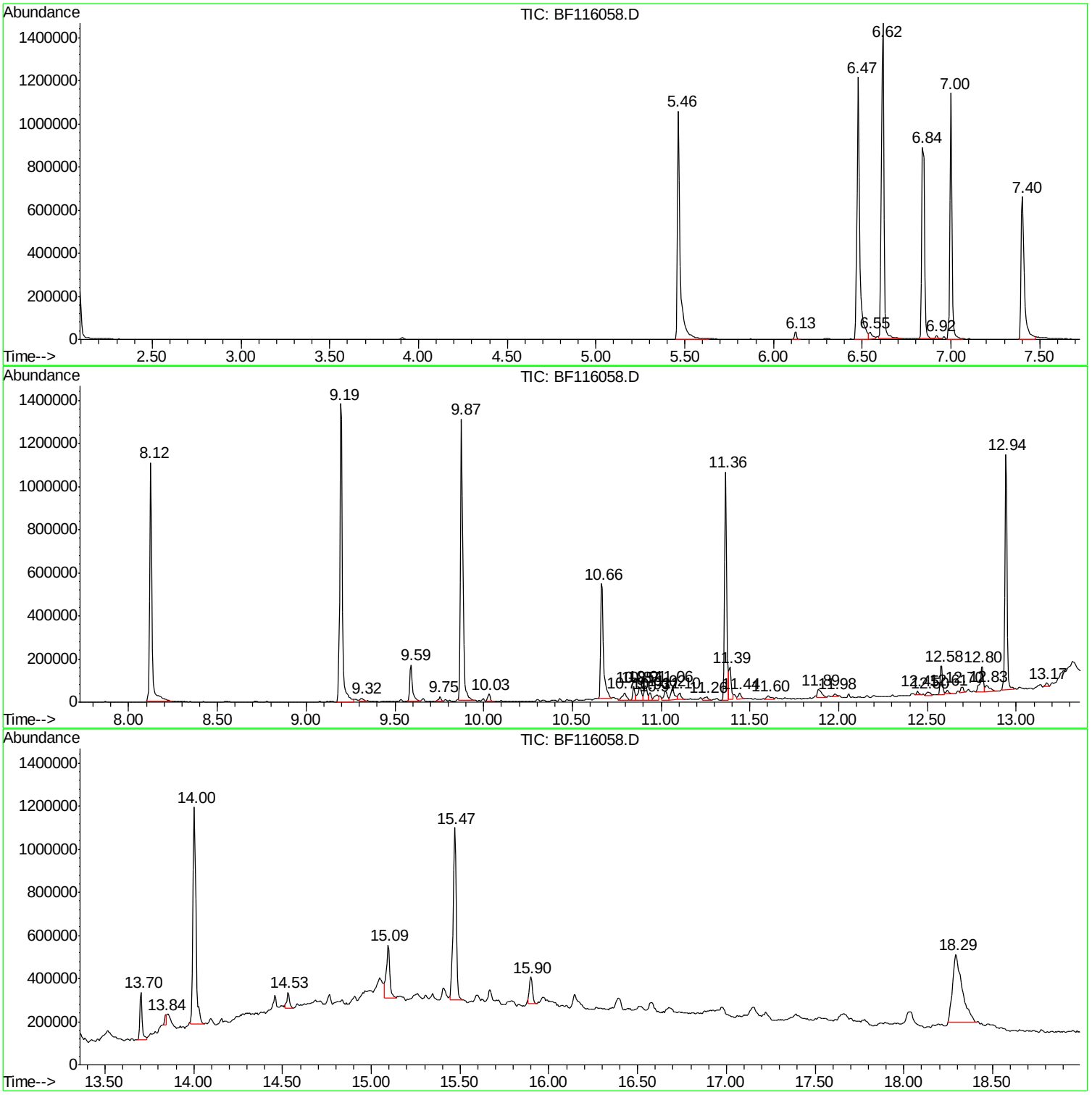
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PS-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080719\
Data File : BF116057.D
Acq On : 7 Aug 2019 20:14
Operator : HP/JU
Sample : K4154-04 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

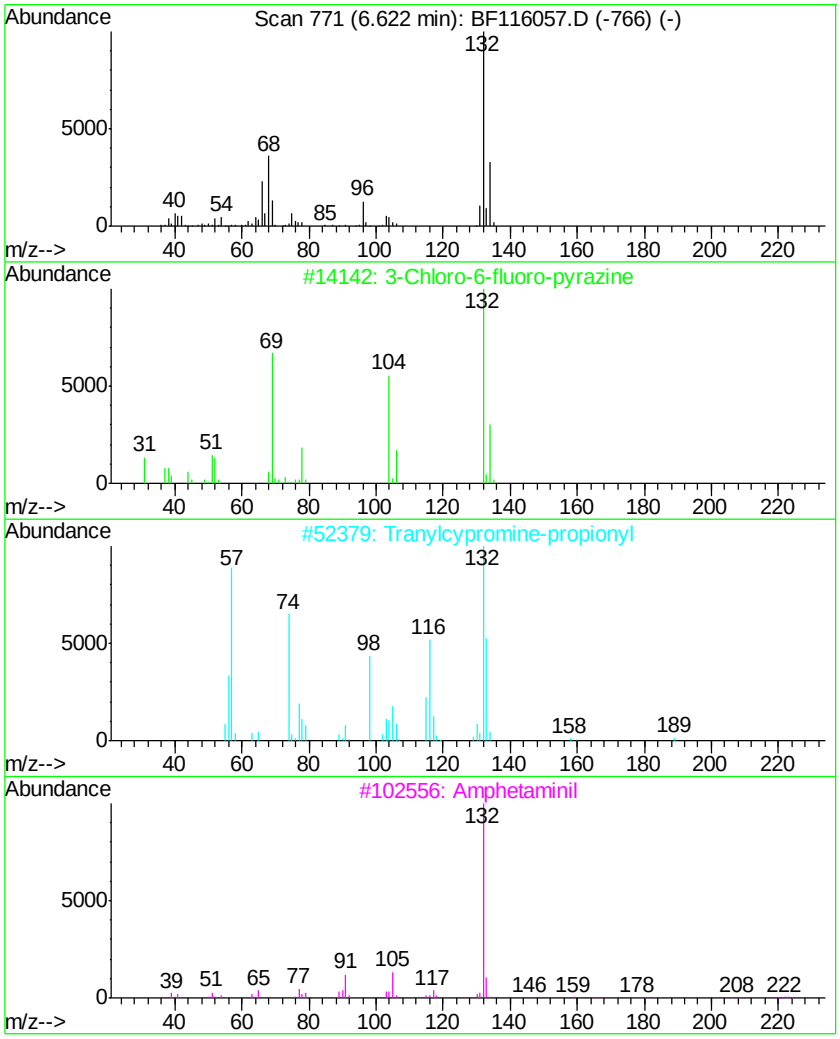
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

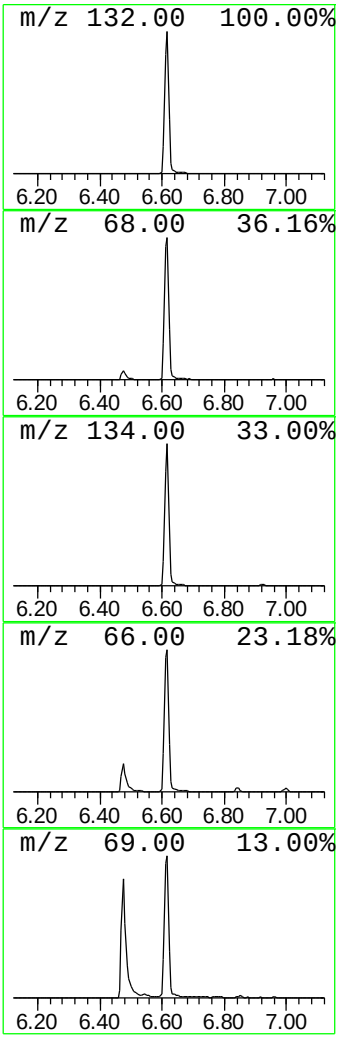
****

Peak Number 1 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	32.27 ng	1378500	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	Amphetaminil	250	C17H18N2	017590-01-1	10
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1H-Indol-4-amine	132	C8H8N2	005192-23-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080719\
Data File : BF116057.D
Acq On : 7 Aug 2019 20:14
Operator : HP/JU
Sample : K4154-04 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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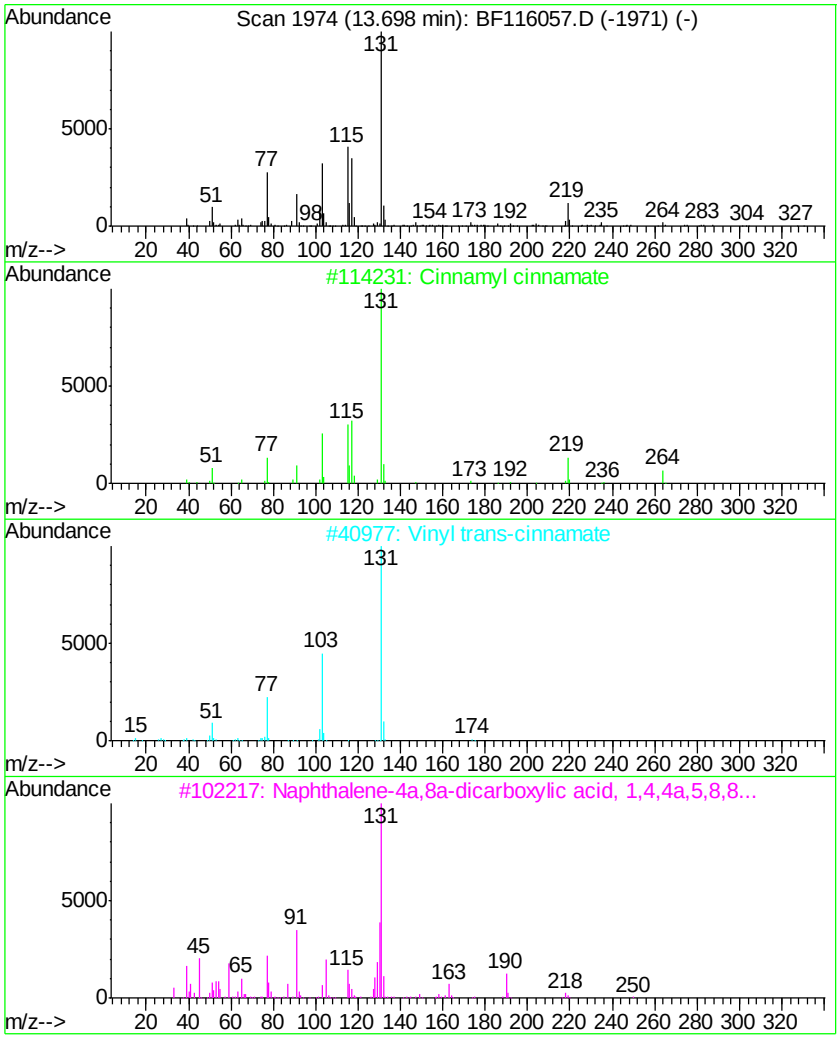
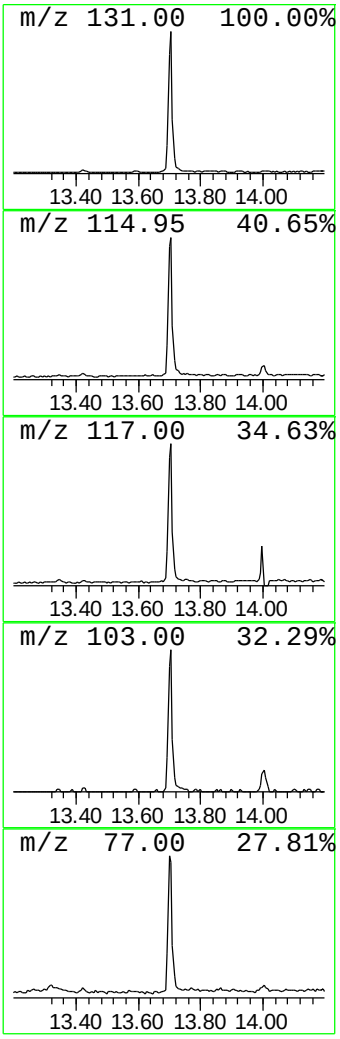
Peak Number 3 Cinnamyl cinnamate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	4.18 ng	221021	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	87
2	Vinyl trans-cinnamate	174	C11H10O2	017719-70-9	64
3	Naphthalene-4a,8a-dicarboxylic a...	250	C14H18O4	007177-20-0	53
4	1-Penten-3-one, 4-methyl-1-phenyl-	174	C12H14O	003160-32-5	50
5	2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	50





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080719\
Data File : BF116057.D
Acq On : 7 Aug 2019 20:14
Operator : HP/JU
Sample : K4154-04 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

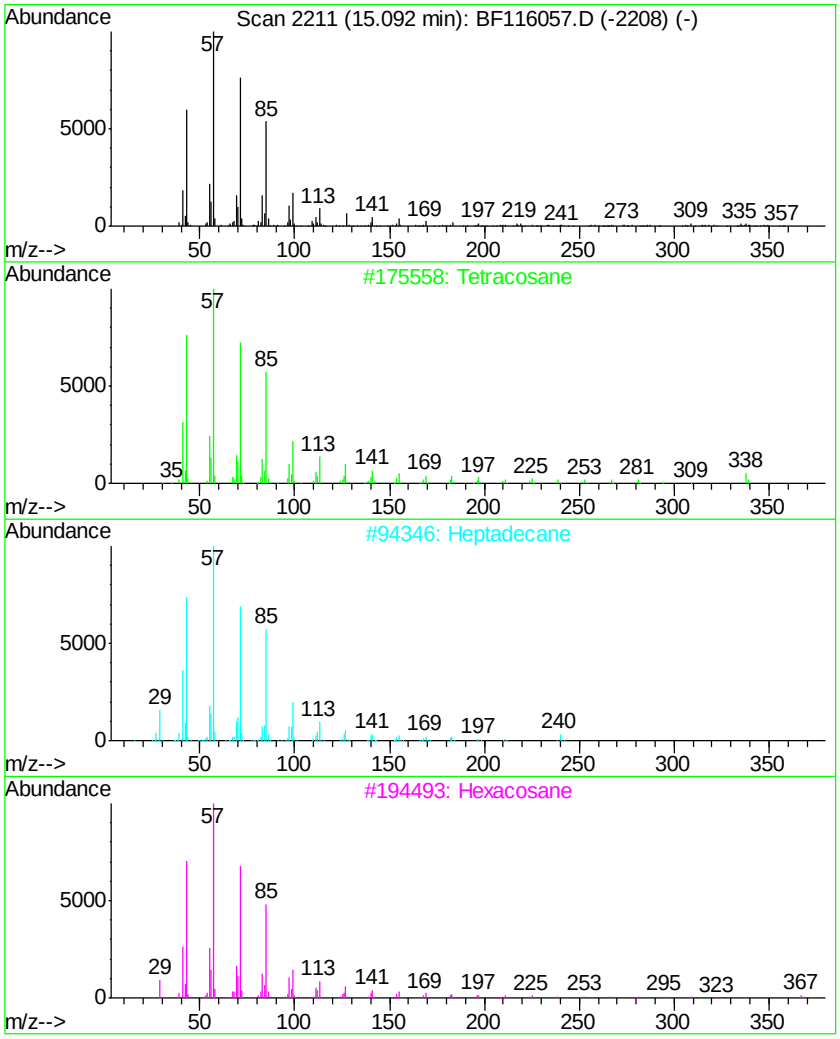
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

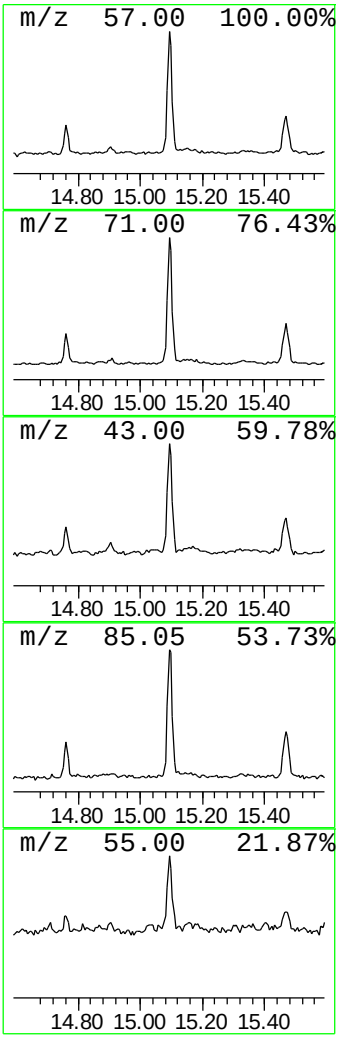
****

Peak Number 4 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	6.24 ng	324831	Perylene-d12	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	97
2	Heptadecane	240	C17H36	000629-78-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Docosane, 5-butyl-	366	C26H54	055282-16-1	90
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080719\
Data File : BF116057.D
Acq On : 7 Aug 2019 20:14
Operator : HP/JU
Sample : K4154-04 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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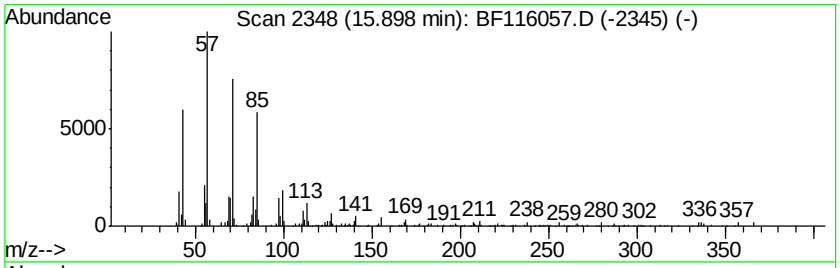
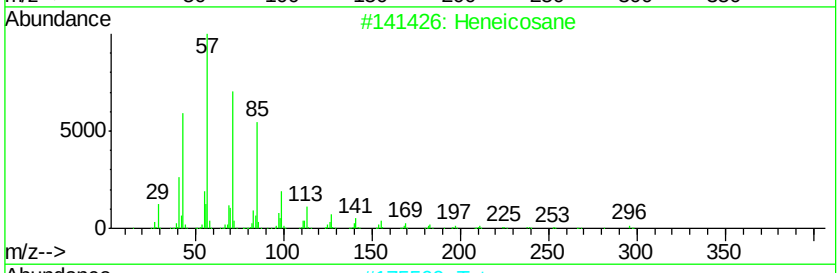
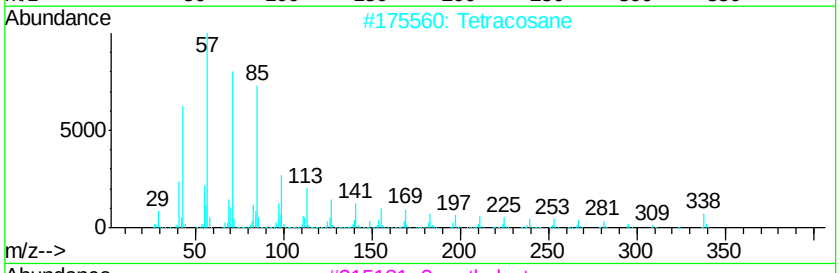
Peak Number 5 Heneicosane Concentration Rank 6

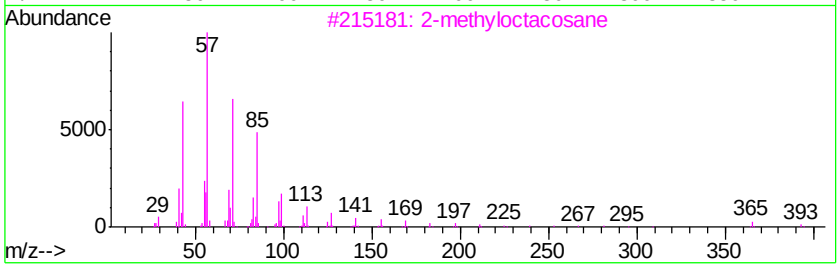
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	3.27 ng	170320	Perylene-d12	15.47

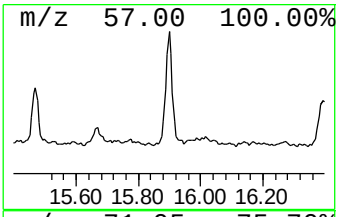
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87

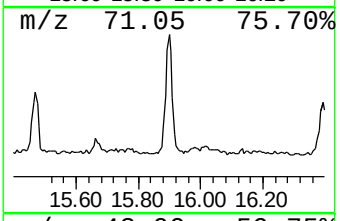


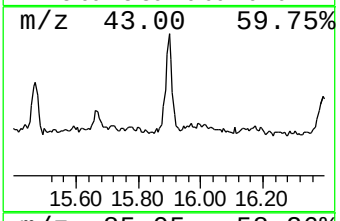


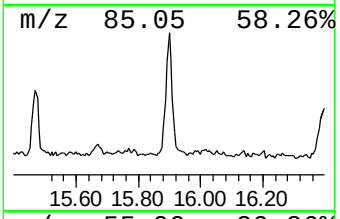


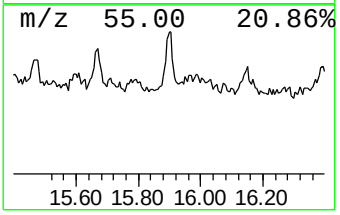












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Data File : BF116057.D
Acq On : 7 Aug 2019 20:14
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Sample : K4154-04 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

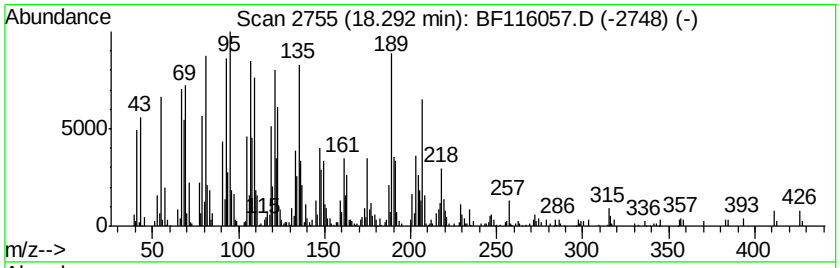
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

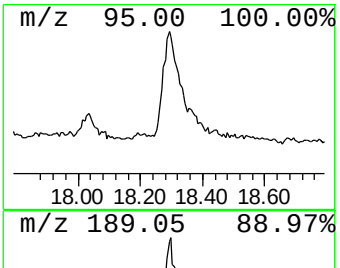
****

Peak Number 6 Hop-22(29)-en-3.beta.-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.29	22.89 ng	1190740	Perylene-d12	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hop-22(29)-en-3.beta.-ol	426	C30H50O	058801-23-3	94
2	1,5,9-Cyclotetradecatriene, 1,5,...	272	C20H32	038748-84-4	74
3	Taraxasterol	426	C30H50O	001059-14-9	56
4	2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	53
5	Guaia-9,11-diene	204	C15H24	1000374-19-8	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080719\
Data File : BF116057.D
Acq On : 7 Aug 2019 20:14
Operator : HP/JU
Sample : K4154-04 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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
unknown6.62	6.62	32.3	ng	1378500	1	6.85	854249	20.0
Cinnamyl cinnamate	13.70	4.2	ng	221021	5	14.00	1058550	20.0
Tetracosane	15.09	6.2	ng	324831	6	15.47	1040390	20.0
Heneicosane	15.90	3.3	ng	170320	6	15.47	1040390	20.0
Hop-22(29)-en-3.b...	18.29	22.9	ng	1190740	6	15.47	1040390	20.0