LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030420\
Data File : BF119207.D
Acq On : 4 Mar 2020 21:21
Operator : CG/JU
Sample : L1772-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-7

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-BF022020.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	5.381	556	560	583	rBV	2598263	2715575	84.66%	11.589%
2	6.404	730	734	755	rBV	2607700	2654743	82.77%	11.329%
3	6.739	788	791	801	rBV	869574	755193	23.54%	3.223%
4	6.898	814	818	822	rBV	2659583	2404216	74.95%	10.260%
5	7.304	883	887	900	rBV	1587755	1709420	53.29%	7.295%
6	8.022	1005	1009	1024	rBV	1077305	926684	28.89%	3.955%
7	9.098	1187	1192	1195	rBV	3592395	3207548	100.00%	13.688%
8	9.492	1256	1259	1267	rVB	137926	125636	3.92%	0.536%
9	9.774	1303	1307	1318	rBV	1064008	950343	29.63%	4.056%
10	10.569	1438	1442	1454	rBV	1792488	1633968	50.94%	6.973%
11	11.263	1556	1560	1565	rBV	823144	800565	24.96%	3.416%
12	11.492	1595	1599	1606	rBV4	21151	34997	1.09%	0.149%
13	11.792	1646	1650	1662	rBV	146366	193141	6.02%	0.824%
14	12.033	1688	1691	1694	rBV	67470	56417	1.76%	0.241%
15	12.574	1780	1783	1789	rBV5	30812	46953	1.46%	0.200%
16	12.839	1824	1828	1832	rBV	2591625	2486227	77.51%	10.610%
17	13.739	1977	1981	1991	rBV	225787	372148	11.60%	1.588%
18	13.898	2004	2008	2012	rBV	769056	758203	23.64%	3.236%
19	14.051	2032	2034	2039	rBV3	30728	49516	1.54%	0.211%
20	14.362	2083	2087	2094	rBV5	73059	192542	6.00%	0.822%
21	14.656	2134	2137	2142	rVB	79034	96846	3.02%	0.413%
22	14.727	2145	2149	2153	rVB	492653	518360	16.16%	2.212%
23	15.209	2229	2231	2236	rVB2	69533	76805	2.39%	0.328%
24	15.333	2248	2252	2259	rVB	533457	666879	20.79%	2.846%

Sum of corrected areas: 23432925

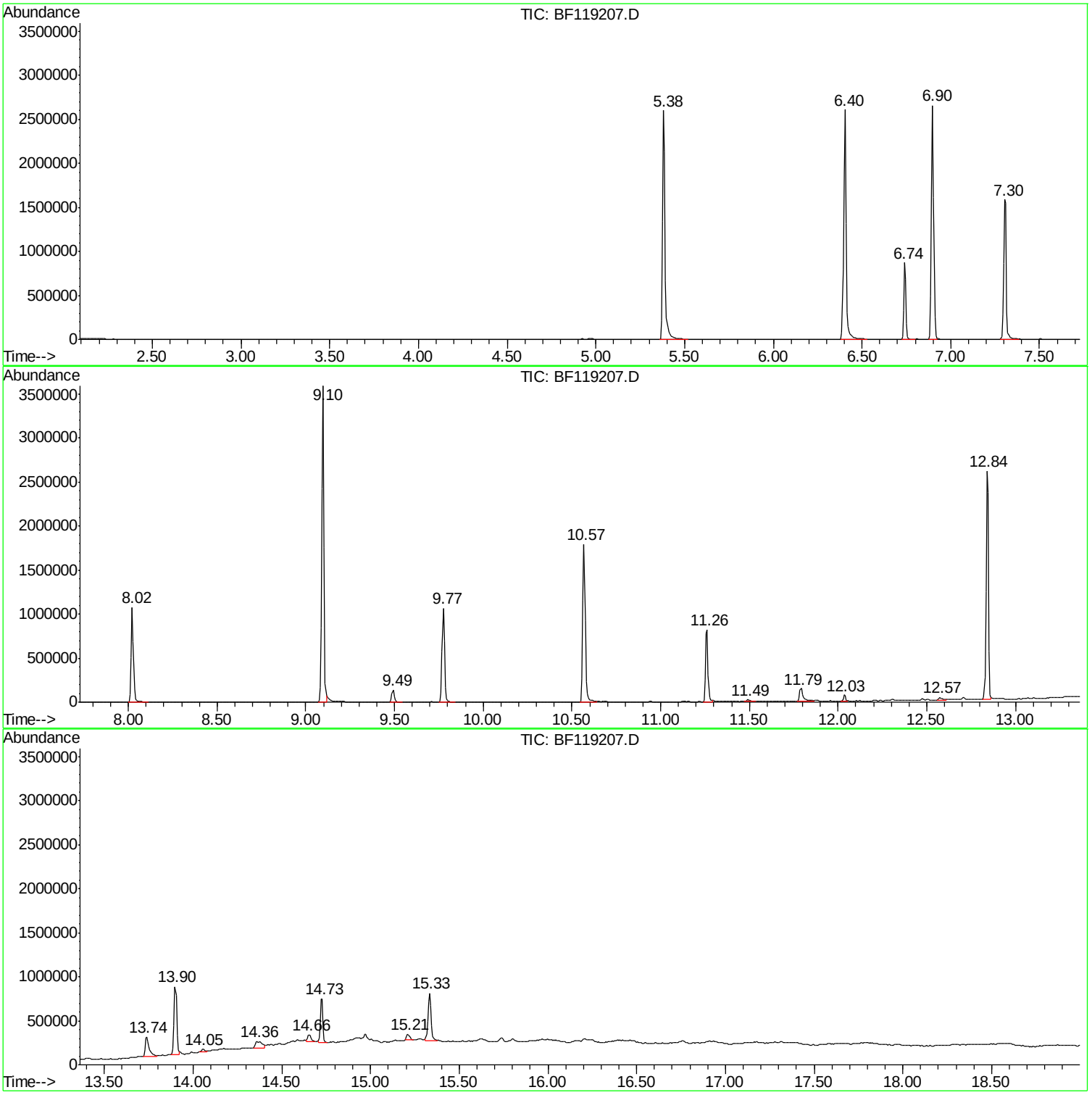
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030420\
Data File : BF119207.D
Acq On : 4 Mar 2020 21:21
Operator : CG/JU
Sample : L1772-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.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\BF030420\
Data File : BF119207.D
Acq On : 4 Mar 2020 21:21
Operator : CG/JU
Sample : L1772-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

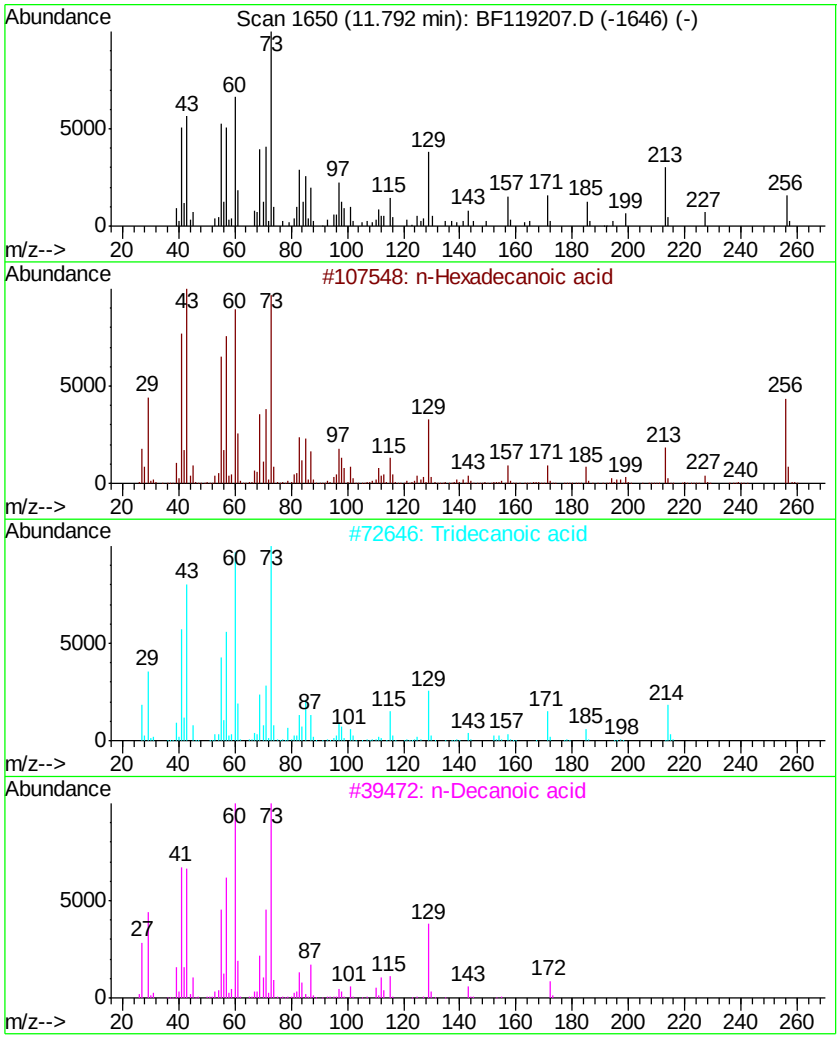
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

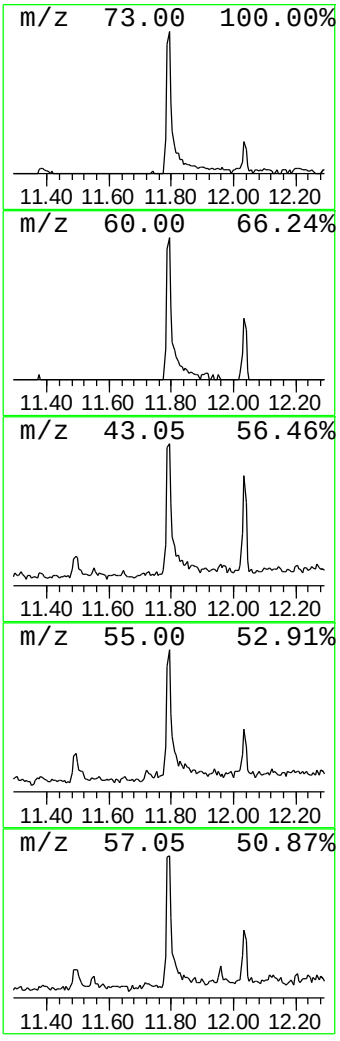
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	4.83 ng	193141	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	n-Decanoic acid	172	C10H20O2	000334-48-5	70
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	25





Library Search Compound Report

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Data File : BF119207.D
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Operator : CG/JU
Sample : L1772-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

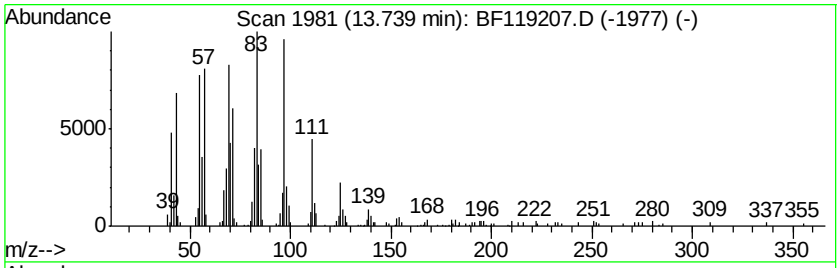
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

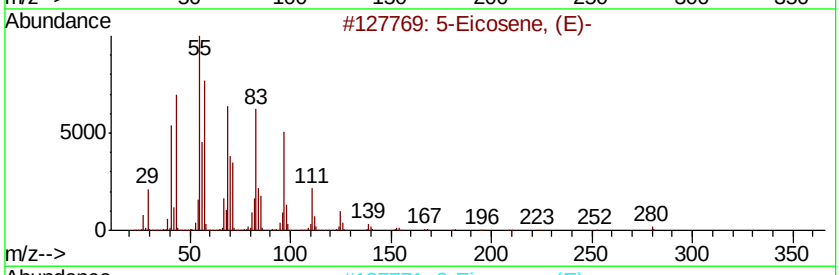
****

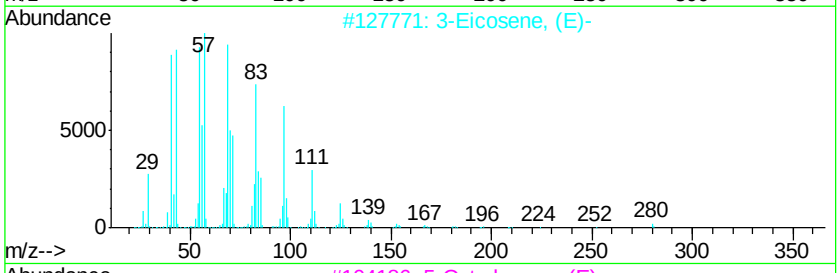
Peak Number 3 5-Eicosene, (E)- Concentration Rank 3

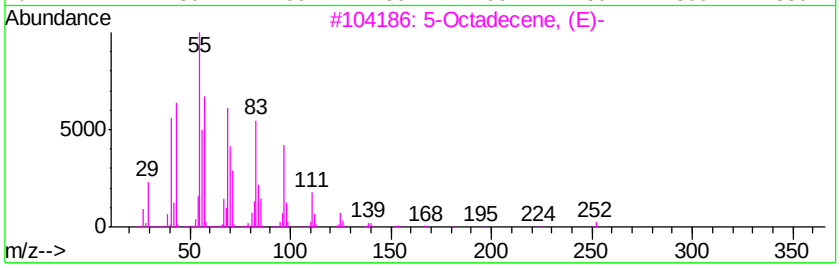
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	9.82 ng	372148	Chrysene-d12	13.90

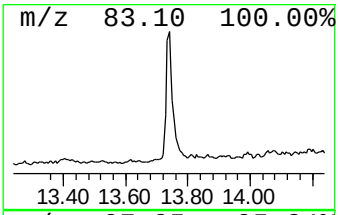
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	98
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	93

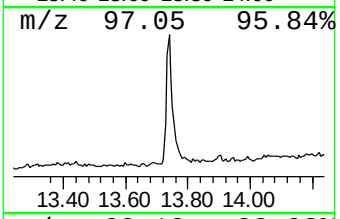


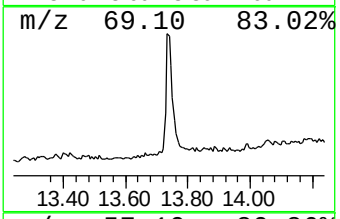


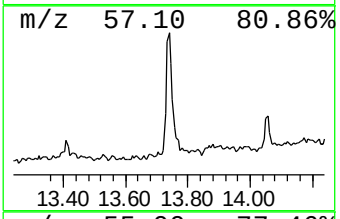


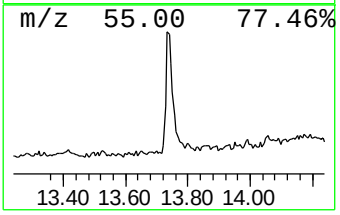












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030420\
Data File : BF119207.D
Acq On : 4 Mar 2020 21:21
Operator : CG/JU
Sample : L1772-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

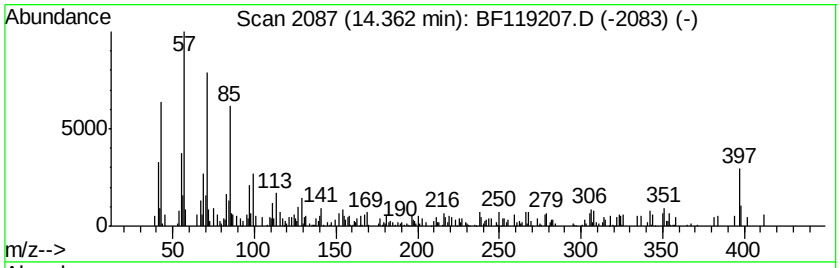
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

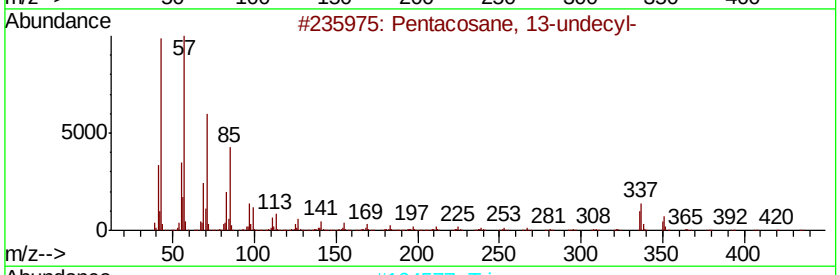
****

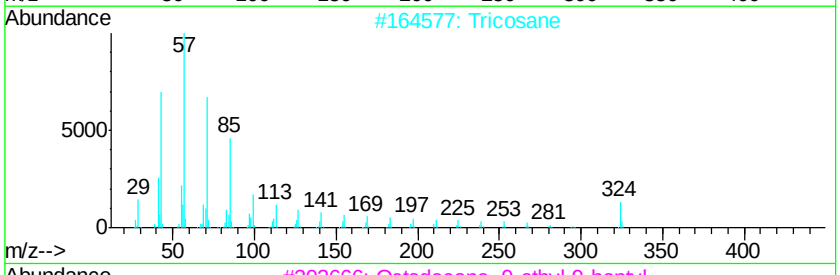
Peak Number 4 Pentacosane, 13-undecyl- Concentration Rank 4

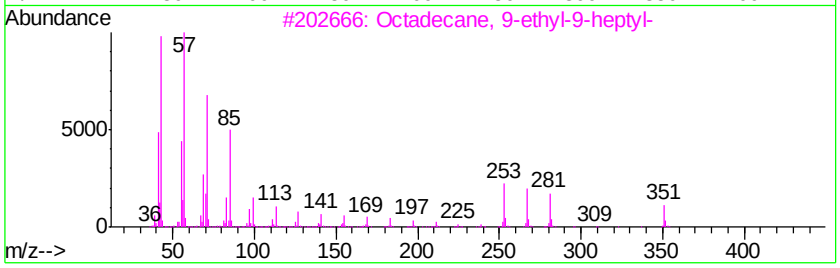
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	5.08 ng	192542	Chrysene-d12	13.90

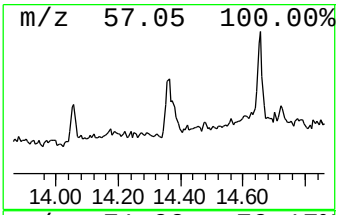
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane, 13-undecyl-	507	C36H74	055517-89-0	64
2	Tricosane	324	C23H48	000638-67-5	53
3	Octadecane, 9-ethyl-9-heptyl-	380	C27H56	055282-27-4	52
4	Tetracosane, 9-octyl-	451	C32H66	055401-54-2	42
5	15,19-Dimethylpentatriacontane	521	C37H76	056987-86-1	42

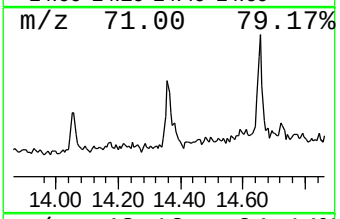


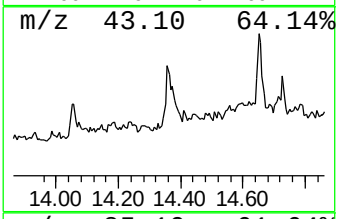


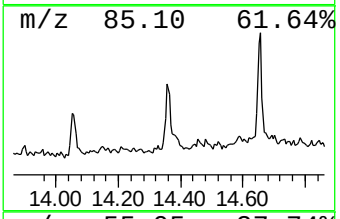


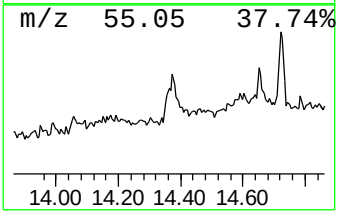












Library Search Compound Report

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Data File : BF119207.D
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Sample : L1772-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

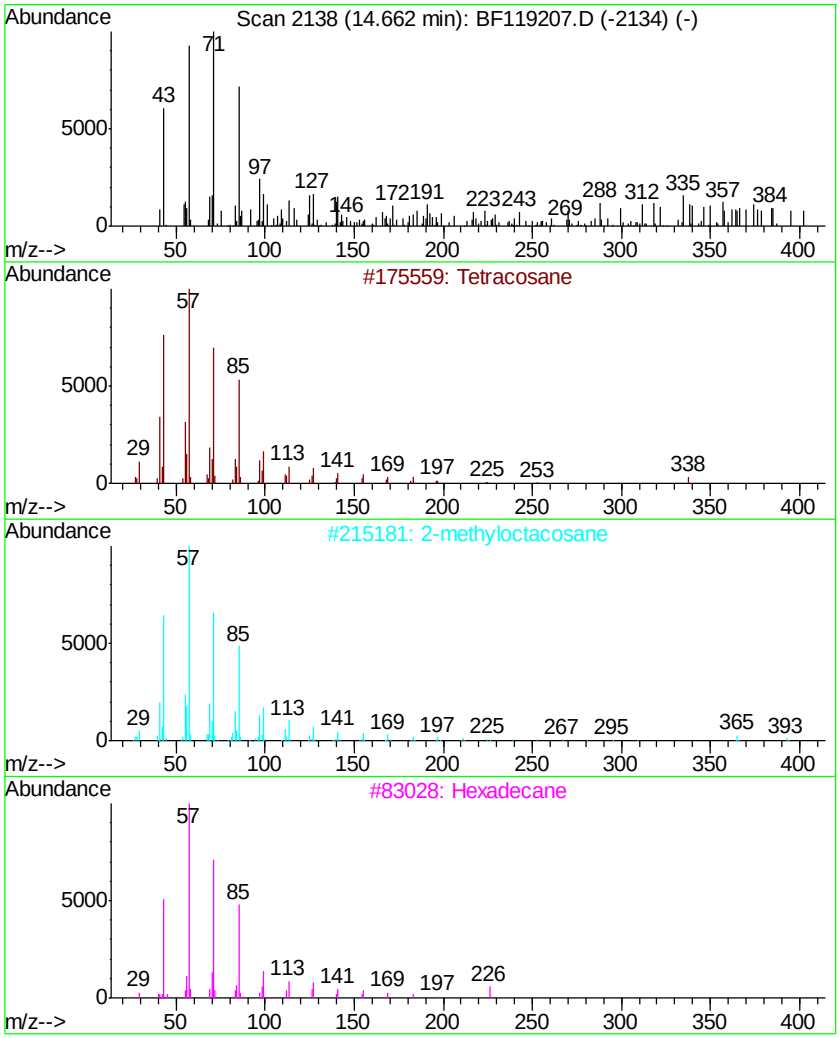
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

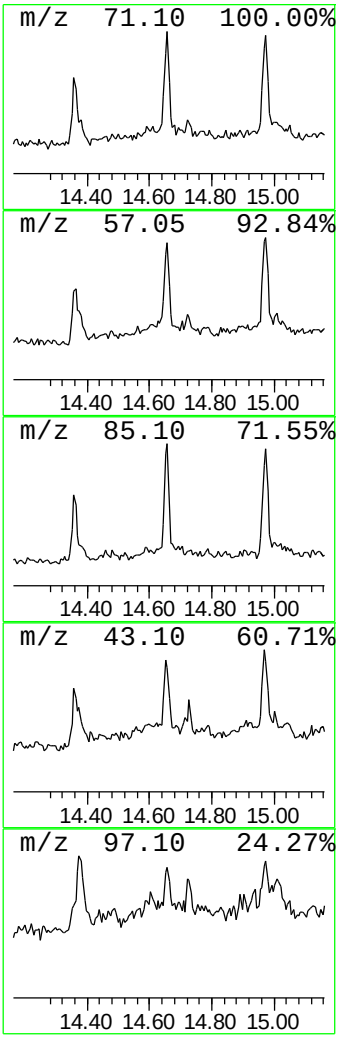
****

Peak Number 5 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	2.90 ng	96846	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	2-methyloctacosane	408	C29H60	1000376-72-8	74
3	Hexadecane	226	C16H34	000544-76-3	72
4	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	72
5	Hexadecane, 3-methyl-	240	C17H36	006418-43-5	64





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Sample : L1772-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

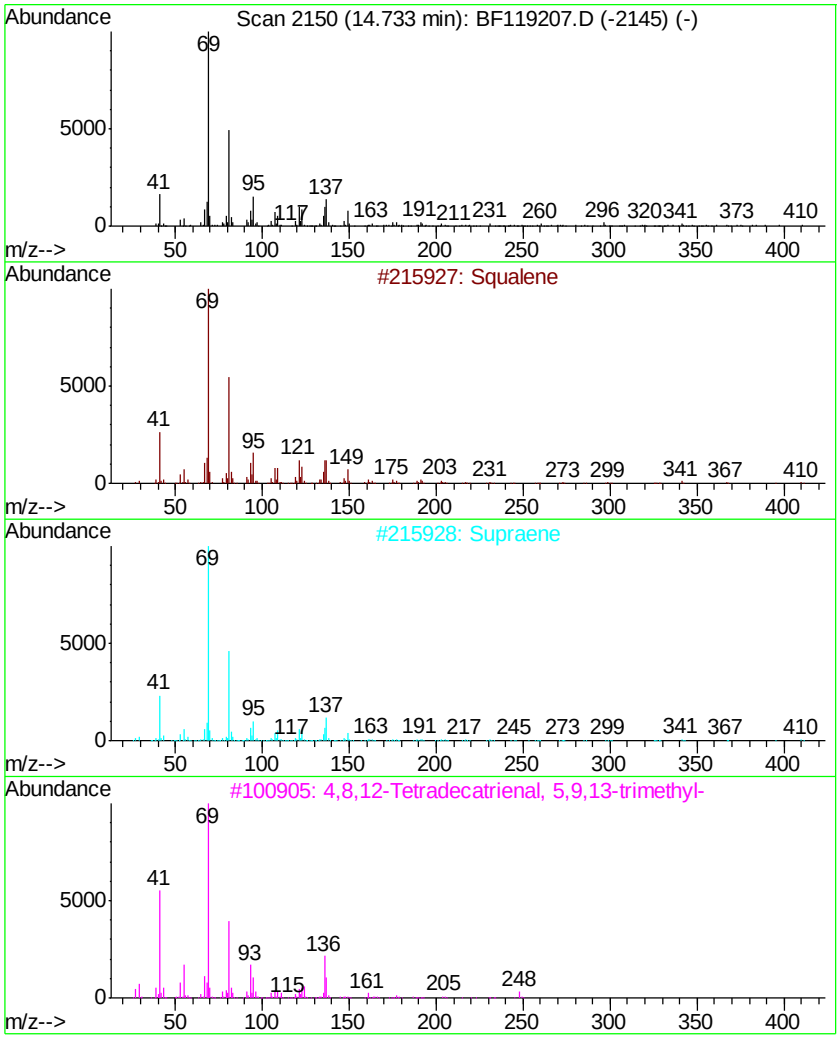
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

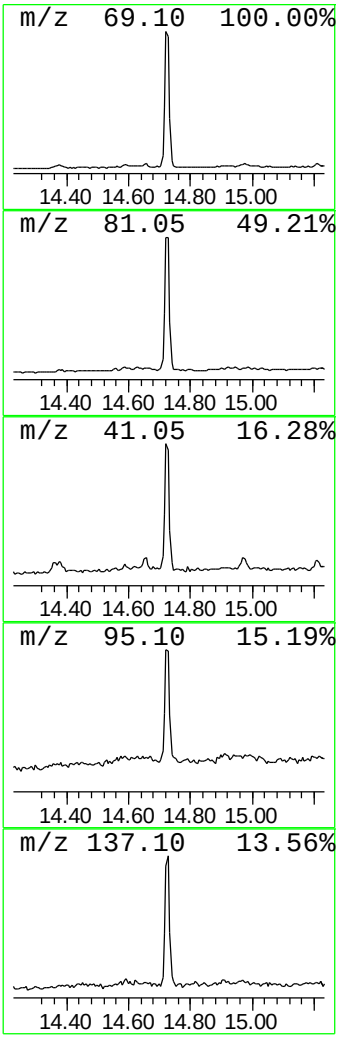
****

Peak Number 6 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	15.55 ng	518360	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	99
2	Supraene	410	C30H50	007683-64-9	96
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5	trans-Farnesol	222	C15H26O	000106-28-5	59





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

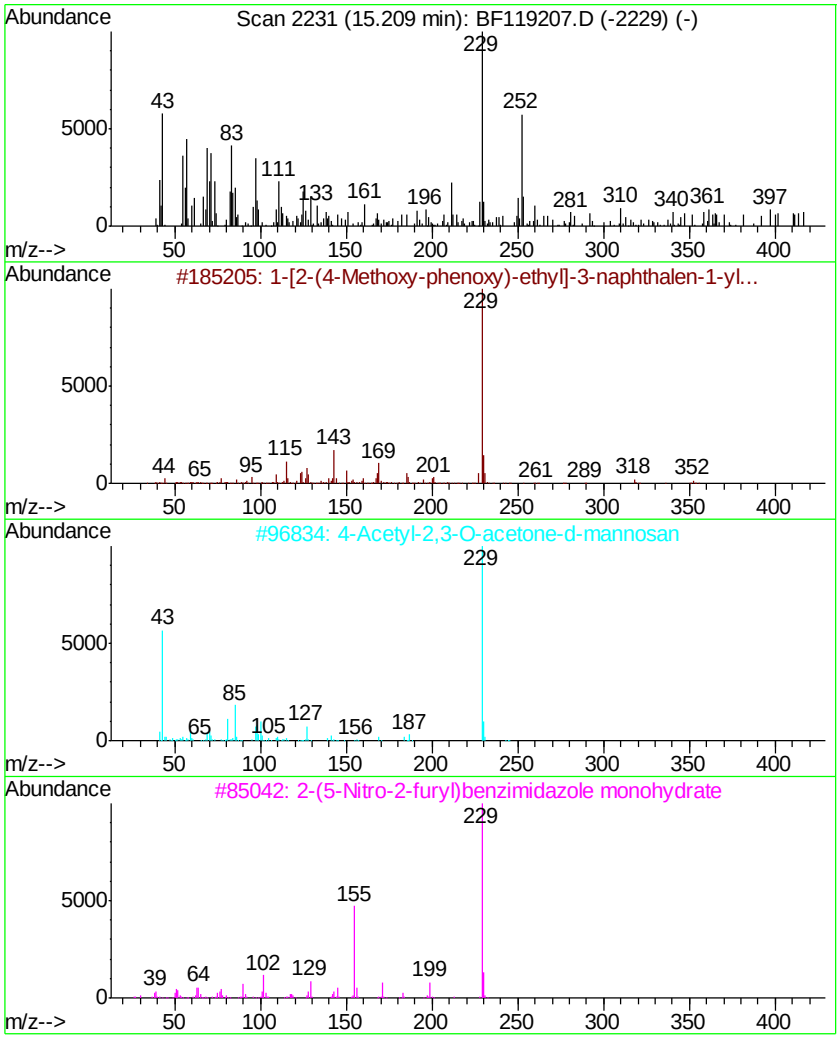
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

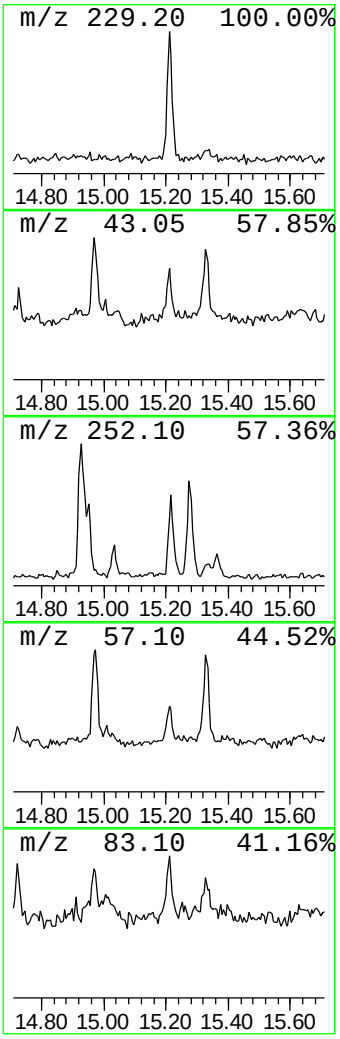
****

Peak Number 7 unknown15.21 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.21	2.30 ng	76805	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-[2-(4-Methoxy-phenoxy)-ethyl]-...	352	C20H20N2O2S	339090-63-0	35
2	4-Acetyl-2,3-O-acetone-d-mannosan	244	C11H16O6	014440-55-2	35
3	2-(5-Nitro-2-furyl)benzimidazole...	229	C11H7N3O3	003945-78-6	35
4	4'-Hydroxyphenazopyridine	229	C11H11N5O	064000-76-6	35
5	5H-1,3,4-Thiadiazolo[3,2-a]pyrim...	229	C7H7N3O2S2	069395-57-9	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030420\
Data File : BF119207.D
Acq On : 4 Mar 2020 21:21
Operator : CG/JU
Sample : L1772-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.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
n-Hexadecanoic acid	11.79	4.8	ng	193141	4	11.26	800565	20.0
5-Eicosene, (E)-	13.74	9.8	ng	372148	5	13.90	758203	20.0
Pentacosane, 13-u...	14.36	5.1	ng	192542	5	13.90	758203	20.0
Tetracosane	14.66	2.9	ng	96846	6	15.33	666879	20.0
Squalene	14.73	15.6	ng	518360	6	15.33	666879	20.0
unknown15.21	15.21	2.3	ng	76805	6	15.33	666879	20.0