LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122222\
Data File : BF131790.D
Acq On : 22 Dec 2022 22:24
Operator : CG\JU
Sample : N6097-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FVSUB-TP1-COMP-01

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-BF122022.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131790.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.063	501	506	515	rVB	635908	794397	37.97%	4.564%
2	5.469	570	575	578	rBV	2004349	1771363	84.67%	10.176%
3	6.487	743	748	751	rBV	1897991	1821980	87.09%	10.467%
4	6.851	807	810	814	rBV	671329	521687	24.94%	2.997%
5	7.422	902	907	910	rBV	1364309	1225686	58.59%	7.041%
6	8.145	1026	1030	1033	rBV	784516	656934	31.40%	3.774%
7	9.222	1209	1213	1216	rBV	2522561	2092014	100.00%	12.018%
8	9.904	1325	1329	1332	rBV	970507	749505	35.83%	4.306%
9	10.551	1432	1439	1442	rBV3	16773	27267	1.30%	0.157%
10	10.622	1446	1451	1455	rVV	48281	46671	2.23%	0.268%
11	10.698	1460	1464	1467	rBV	1504960	1271830	60.79%	7.307%
12	10.816	1480	1484	1490	rBV2	43554	60355	2.89%	0.347%
13	11.286	1561	1564	1571	rVB3	36760	43987	2.10%	0.253%
14	11.398	1579	1583	1585	rBV	858413	695012	33.22%	3.993%
15	11.422	1585	1587	1590	rVV	199757	150948	7.22%	0.867%
16	11.469	1593	1595	1598	rVB	42526	36144	1.73%	0.208%
17	11.627	1620	1622	1627	rVB3	22878	24442	1.17%	0.140%
18	11.898	1665	1668	1670	rBV	30811	31328	1.50%	0.180%
19	11.922	1670	1672	1676	rVV2	176778	167607	8.01%	0.963%
20	12.010	1684	1687	1690	rBV2	51502	55004	2.63%	0.316%
21	12.451	1759	1762	1765	rBV	31712	35749	1.71%	0.205%
22	12.539	1774	1777	1783	rVB3	24113	28915	1.38%	0.166%
23	12.616	1786	1790	1794	rVB	368377	330395	15.79%	1.898%
24	12.845	1823	1829	1834	rBV	330755	357039	17.07%	2.051%
25	12.892	1835	1837	1841	rVB3	23021	28208	1.35%	0.162%
26	12.986	1849	1853	1859	rVB	1666958	1436651	68.67%	8.253%
27	13.057	1862	1865	1870	rVB4	26408	39040	1.87%	0.224%
28	13.151	1878	1881	1882	rBV2	24420	28248	1.35%	0.162%
29	13.174	1882	1885	1888	rVB	47465	48713	2.33%	0.280%
30	13.274	1899	1902	1905	rVB2	42432	39973	1.91%	0.230%
31	13.368	1915	1918	1921	rVB	32265	27479	1.31%	0.158%
32	13.398	1921	1923	1926	rBV2	26130	28030	1.34%	0.161%
33	13.680	1968	1971	1975	rVB	36921	41060	1.96%	0.236%
34	13.792	1986	1990	1993	rBV3	33857	41312	1.97%	0.237%
35	13.845	1997	1999	2004	rBV2	25176	35261	1.69%	0.203%
36	13.892	2004	2007	2017	rBV5	75094	161765	7.73%	0.929%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122222\
Data File : BF131790.D
Acq On : 22 Dec 2022 22:24
Operator : CG\JU
Sample : N6097-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FVSUB-TP1-COMP-01

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-BF122022.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.045	2026	2033	2036	rBV2	571008	691529	33.06%	3.973%
38	14.074	2036	2038	2045	rVB	162110	148520	7.10%	0.853%
39	14.145	2045	2050	2053	rBV2	114491	143520	6.86%	0.825%
40	14.433	2097	2099	2102	rVB	44440	34176	1.63%	0.196%
41	14.810	2160	2163	2168	rVB4	34748	48379	2.31%	0.278%
42	14.898	2174	2178	2181	rBV	114732	121880	5.83%	0.700%
43	15.098	2208	2212	2215	rBV	165390	239973	11.47%	1.379%
44	15.168	2222	2224	2228	rVB2	29606	28874	1.38%	0.166%
45	15.210	2228	2231	2235	rBV	29963	35298	1.69%	0.203%
46	15.410	2261	2265	2271	rVB	97061	124304	5.94%	0.714%
47	15.468	2271	2275	2281	rBV	135299	167111	7.99%	0.960%
48	15.539	2282	2287	2290	rBV	363829	471561	22.54%	2.709%
49	17.033	2535	2541	2551	rVB2	53564	116223	5.56%	0.668%
50	17.486	2613	2618	2625	rVB2	40569	83351	3.98%	0.479%

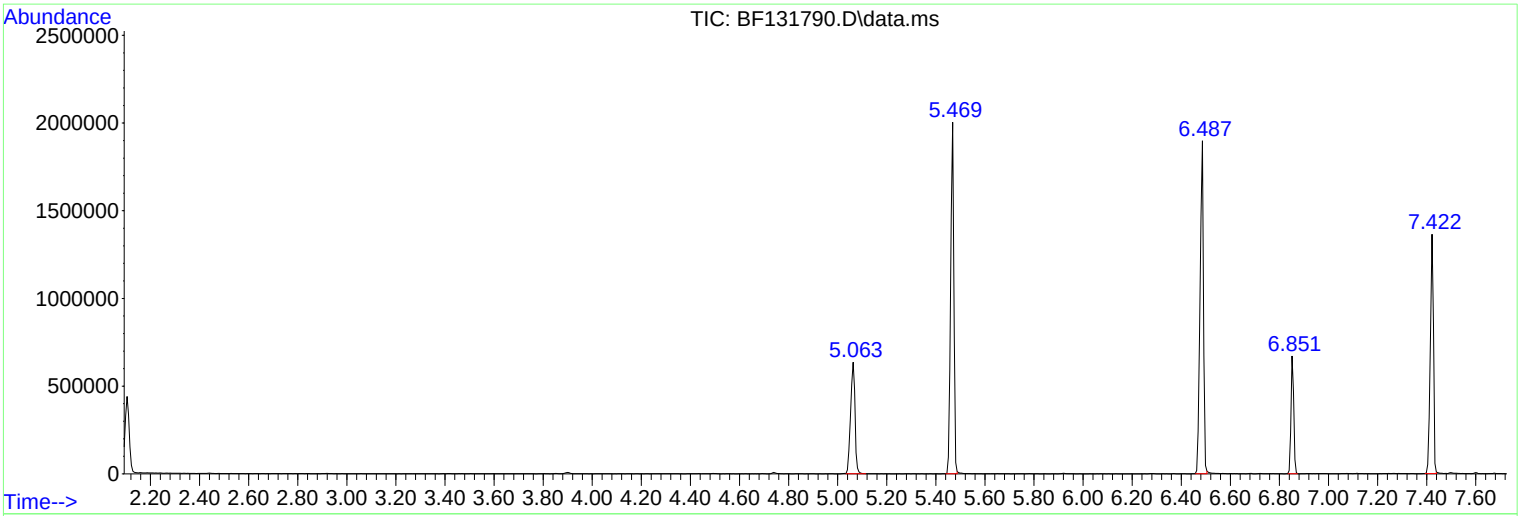
Sum of corrected areas: 17406698

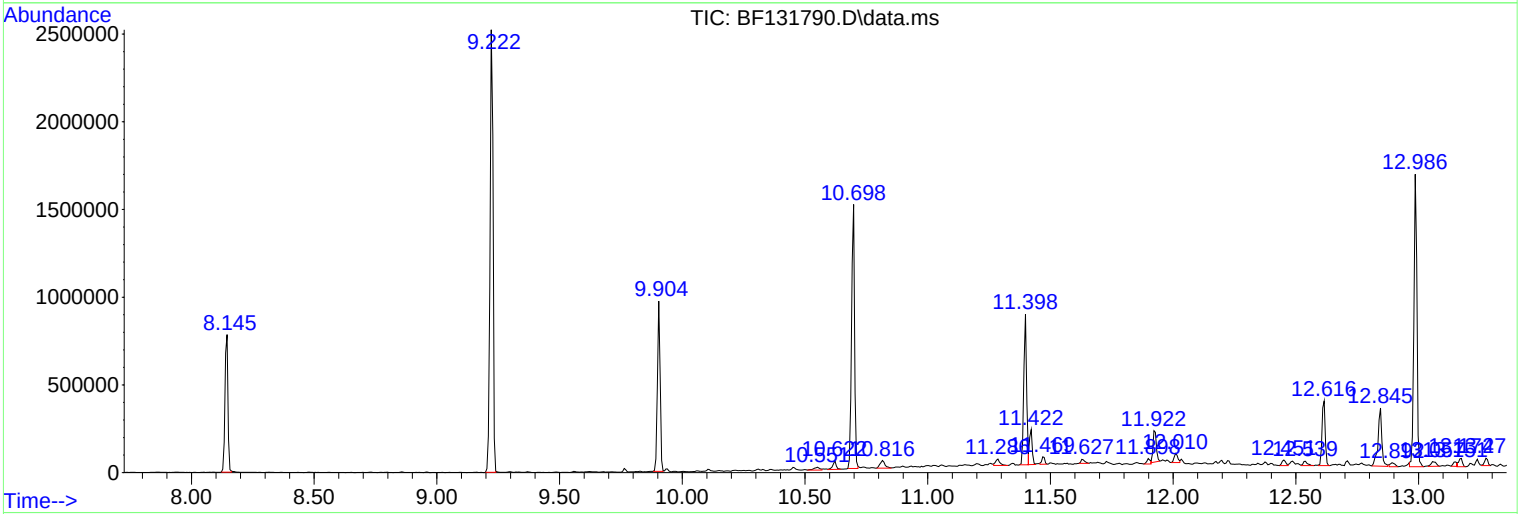
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122222\
Data File : BF131790.D
Acq On : 22 Dec 2022 22:24
Operator : CG\JU
Sample : N6097-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

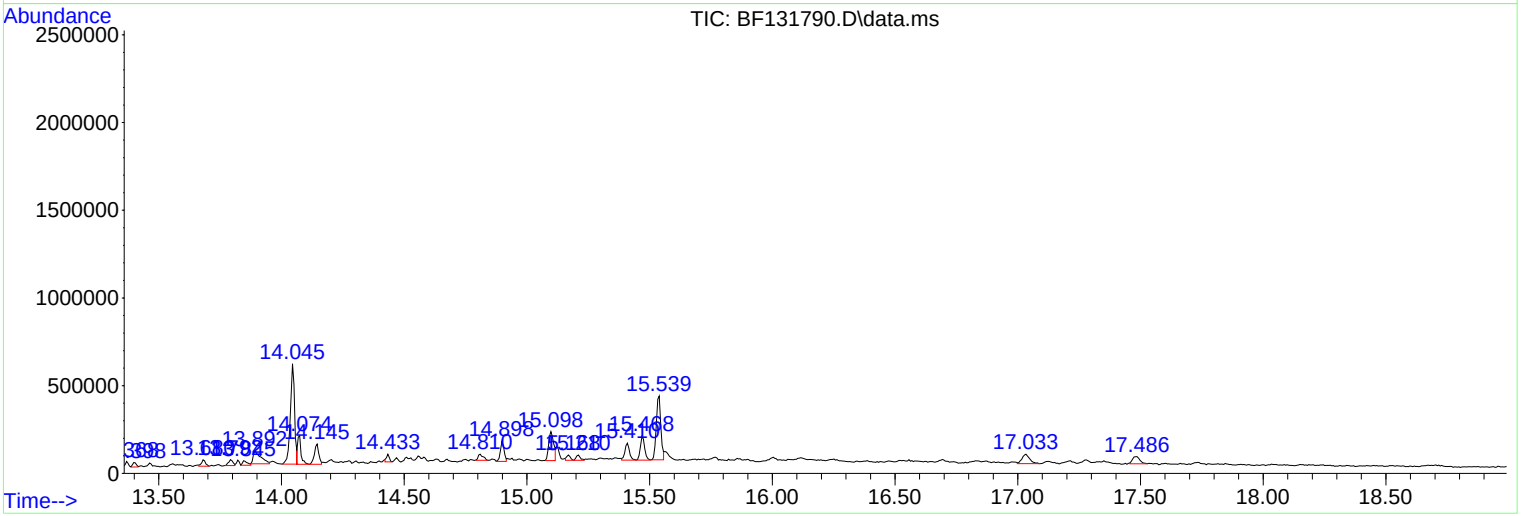
Instrument :
BNA_F
ClientSampleId :
FVSUB-TP1-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122222\
Data File : BF131790.D
Acq On : 22 Dec 2022 22:24
Operator : CG\JU
Sample : N6097-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FVSUB-TP1-COMP-01

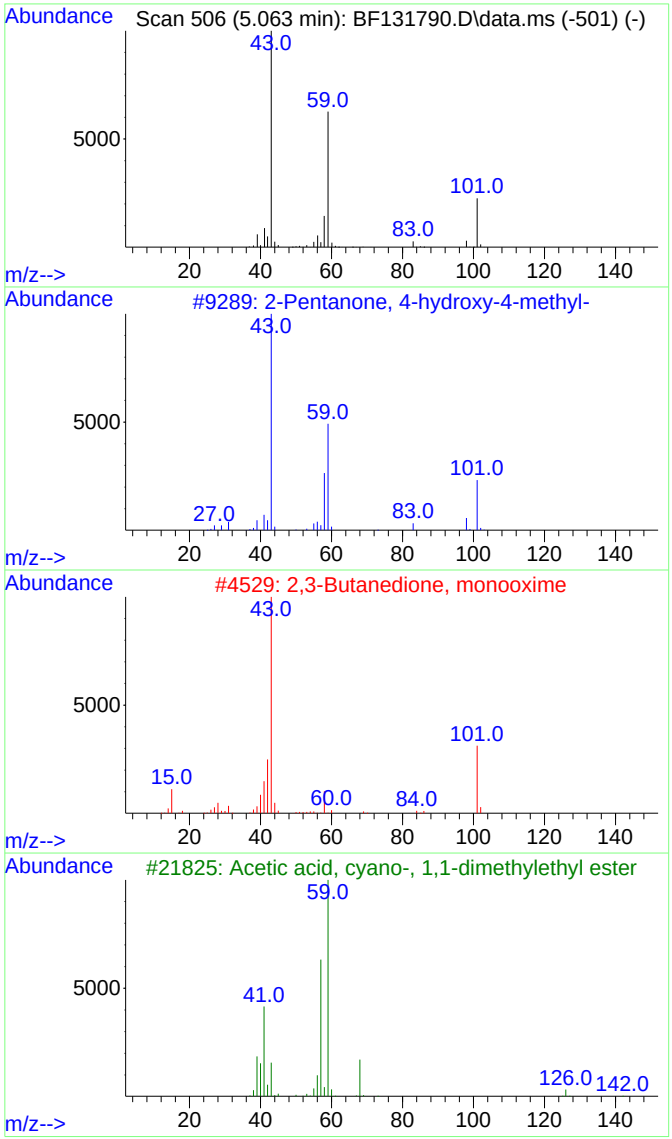
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

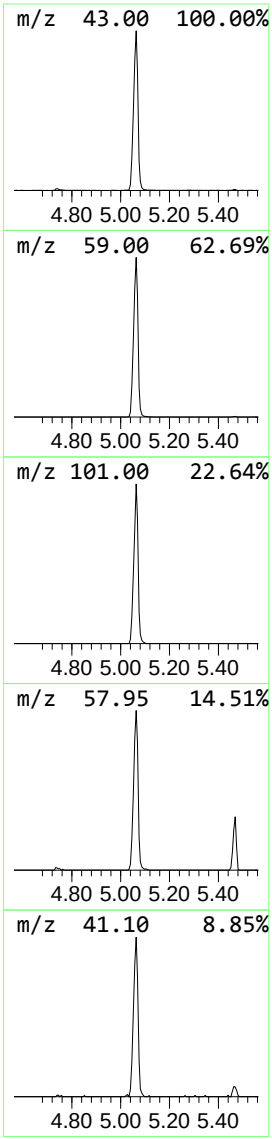
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	30.45 ng	794397	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122222\
Data File : BF131790.D
Acq On : 22 Dec 2022 22:24
Operator : CG\JU
Sample : N6097-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FVSUB-TP1-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

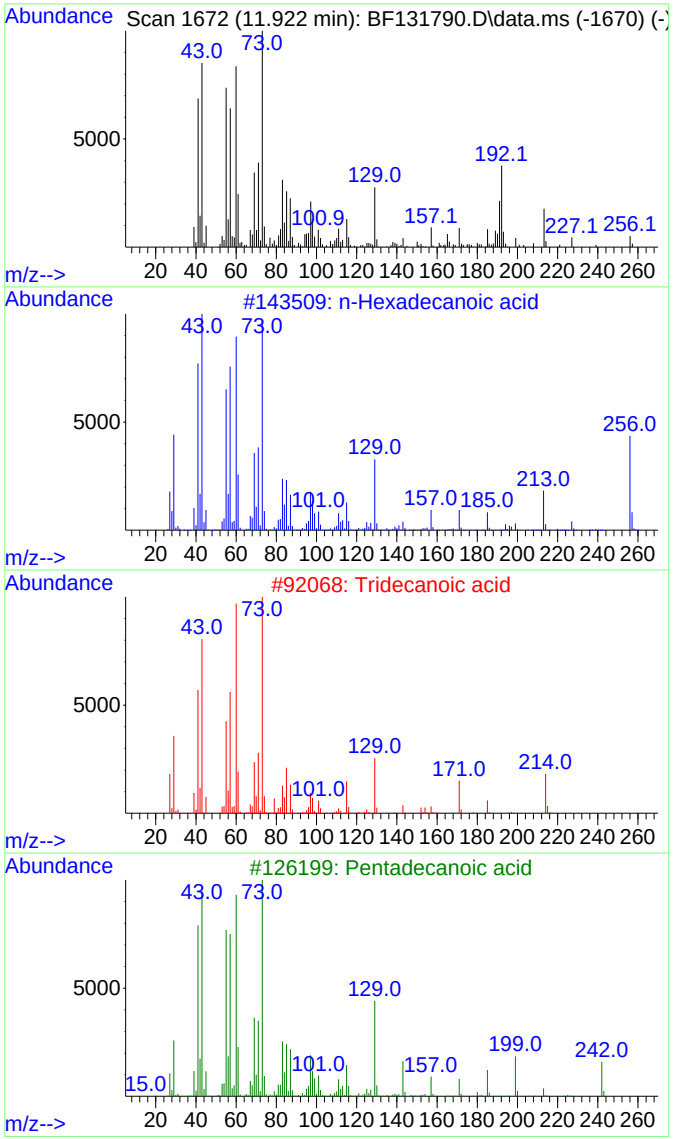
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

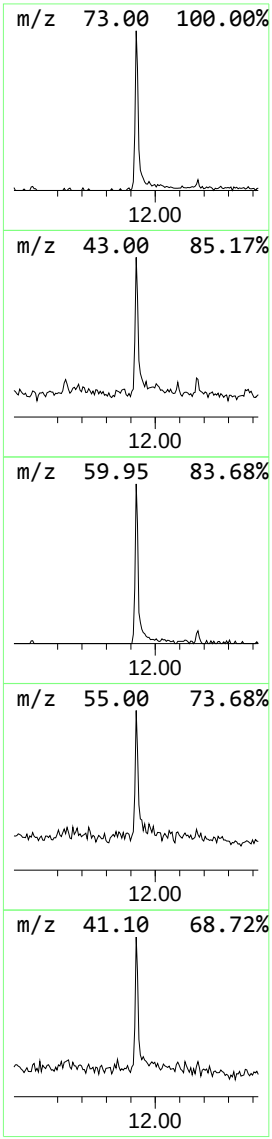
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	4.82 ng	167607	Phenanthrene-d10	11.398

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	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122222\
Data File : BF131790.D
Acq On : 22 Dec 2022 22:24
Operator : CG\JU
Sample : N6097-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FVSUB-TP1-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

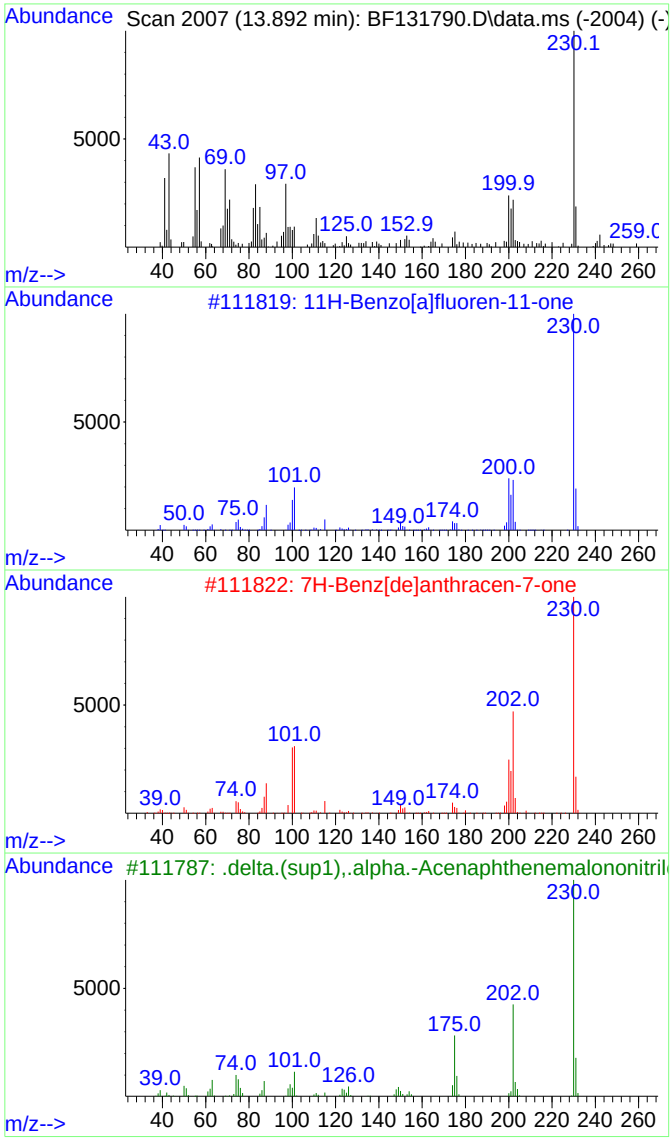
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

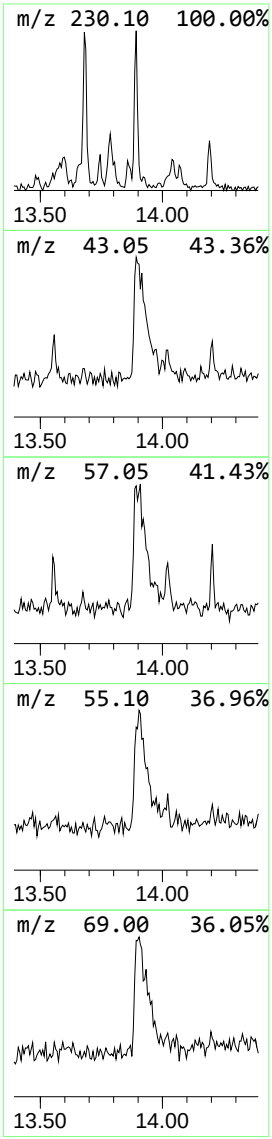
****

Peak Number 3 11H-Benzo[a]fluoren-11-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	4.68 ng	161765	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	76
2	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	70
3	.delta.(sup1),.alpha.-Acenaphthe...	230	C15H6N2O	014619-86-4	58
4	2-Chloro-9-xanthenone	230	C13H7ClO2	013210-15-6	43
5	p-Terphenyl	230	C18H14	000092-94-4	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122222\
Data File : BF131790.D
Acq On : 22 Dec 2022 22:24
Operator : CG\JU
Sample : N6097-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FVSUB-TP1-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

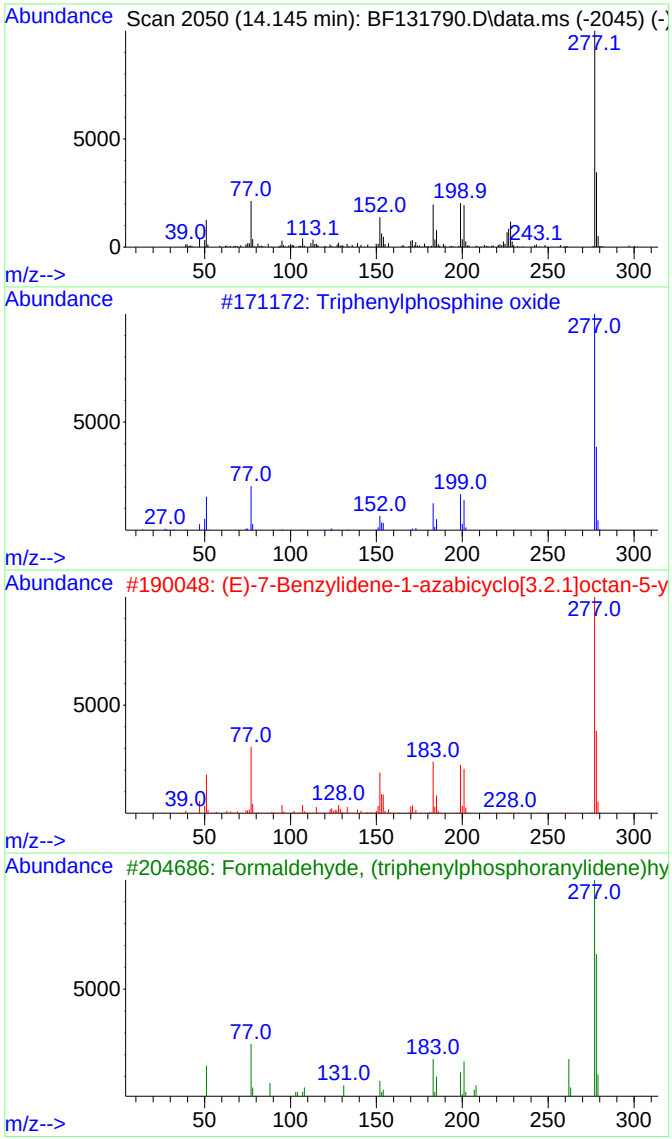
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

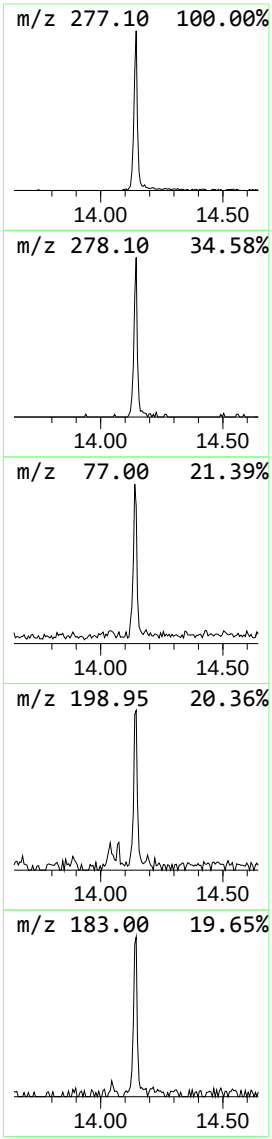
****

Peak Number 4 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.145	4.15 ng	143520	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	98
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4	4-Cyano-8-trifluoromethylnaphtho...	277	C14H6F3NS	037094-50-1	35
5	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122222\
Data File : BF131790.D
Acq On : 22 Dec 2022 22:24
Operator : CG\JU
Sample : N6097-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FVSUB-TP1-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

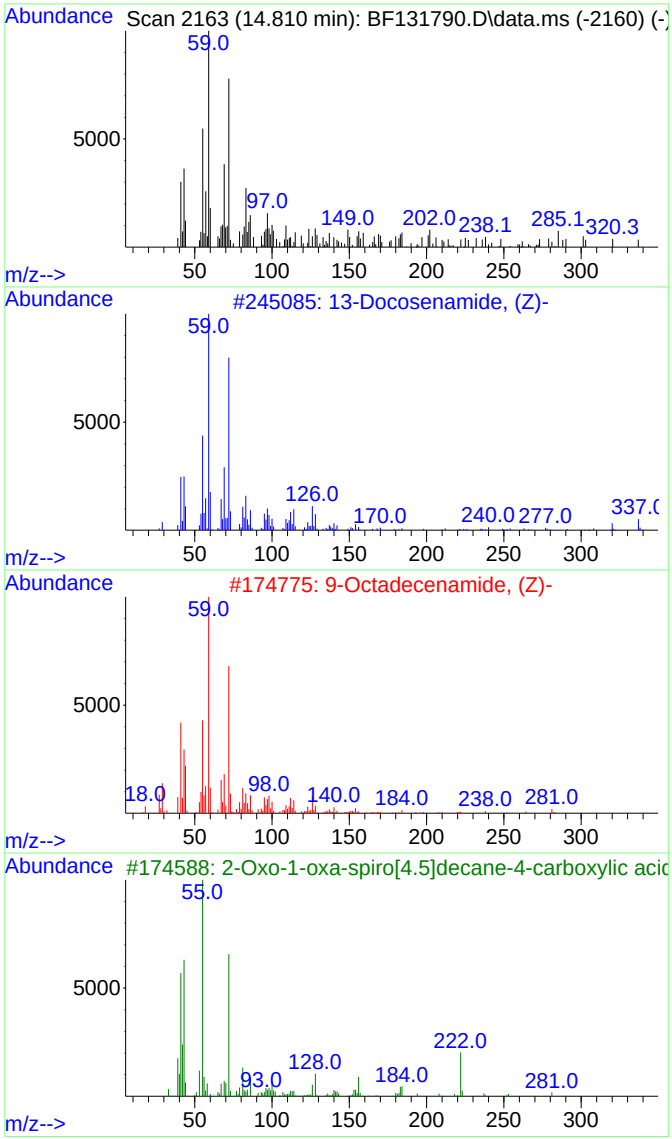
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

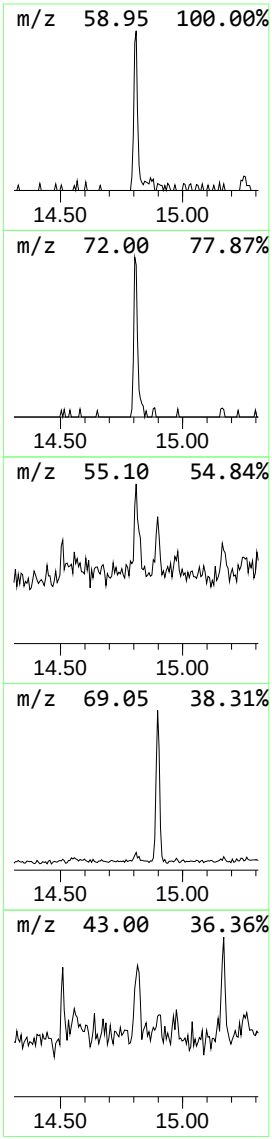
****

Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.810	2.05 ng	48379	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	74
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	72
3	2-Oxo-1-oxa-spiro[4.5]decane-4-c...	281	C16H27NO3	1010300-07-1	42
4	Hept-4-enoylamide, N-(2-butyl)-N...	211	C13H25NO	1000491-70-1	38
5	Hexanamide, 2-ethyl-N-(2-butyl)-...	227	C14H29NO	1000490-92-2	38





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Acq On : 22 Dec 2022 22:24
Operator : CG\JU
Sample : N6097-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FVSUB-TP1-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

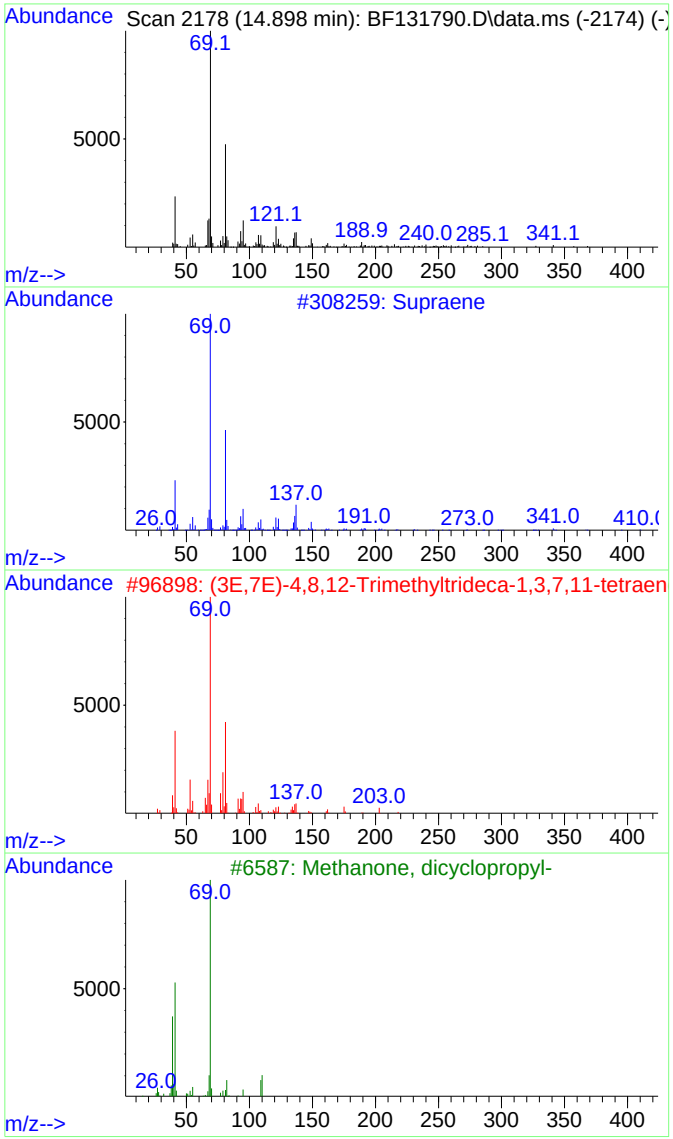
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

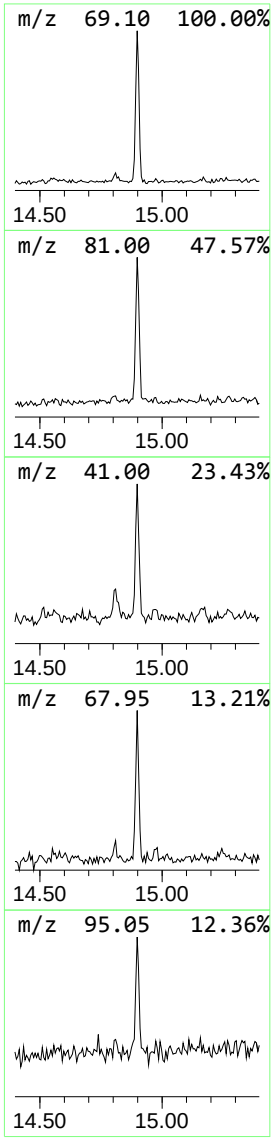
****

Peak Number 6 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	5.17 ng	121880	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	80
2	(3E,7E)-4,8,12-Trimethyltrideca-...	218	C16H26	062235-06-7	76
3	Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	47
4	2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	47
5	1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122222\
Data File : BF131790.D
Acq On : 22 Dec 2022 22:24
Operator : CG\JU
Sample : N6097-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FVSUB-TP1-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

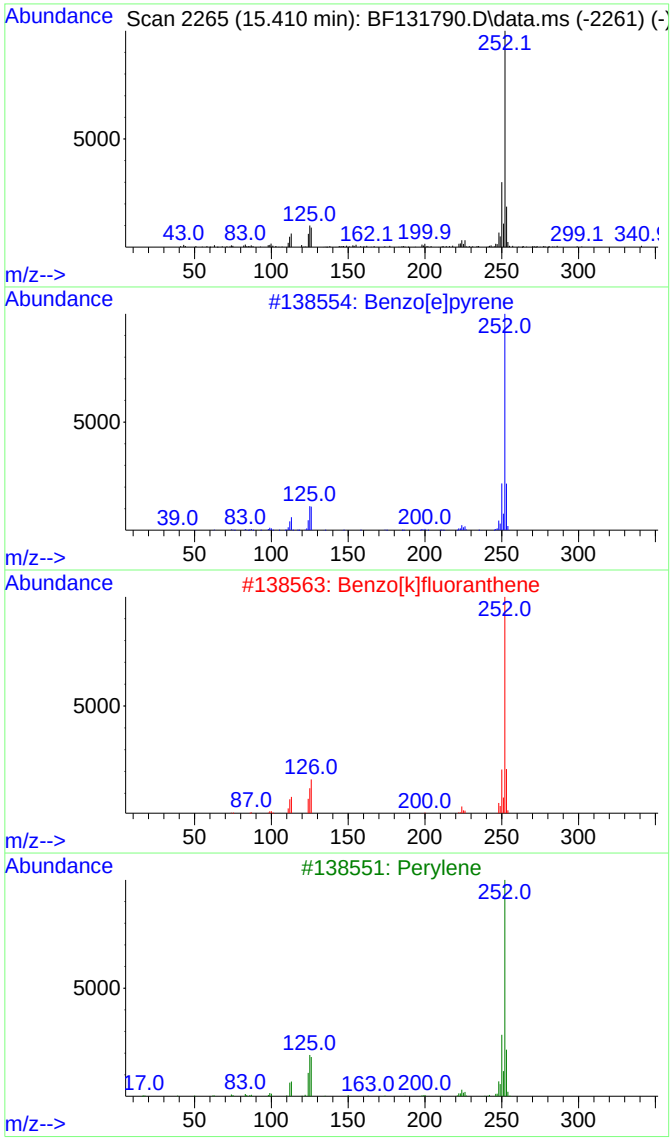
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

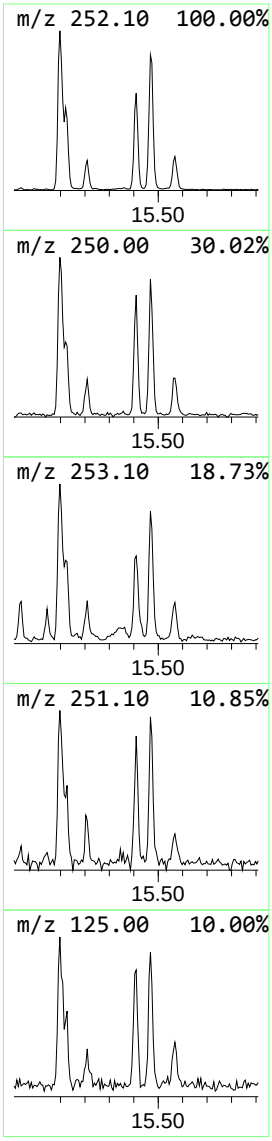
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	5.27 ng	124304	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Perylene	252	C20H12	000198-55-0	95
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122222\
Data File : BF131790.D
Acq On : 22 Dec 2022 22:24
Operator : CG\JU
Sample : N6097-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FVSUB-TP1-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.063	30.4	ng	794397	1	6.851	521687	20.0
n-Hexadecanoic ...	11.922	4.8	ng	167607	4	11.398	695012	20.0
11H-Benzo[a]flu...	13.892	4.7	ng	161765	5	14.045	691529	20.0
Triphenylphosph...	14.145	4.2	ng	143520	5	14.045	691529	20.0
13-Docosenamide...	14.810	2.0	ng	48379	6	15.539	471561	20.0
Supraene	14.898	5.2	ng	121880	6	15.539	471561	20.0
Benzo[e]pyrene	15.410	5.3	ng	124304	6	15.539	471561	20.0